

GEMSS

Grid-enabled Medical Simulation Services

<http://www.gemss.de>

Deliverable D6.3b Edited Final Report

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The GEMSS Consortium:

NEC Europe Ltd. – UK
ISS – Austria
CRID – Belgium
ASD – Germany
IT-Innovation – UK

MPI of Cognitive Neuroscience – Germany
IBMTP – Austria
ANSYS – UK
IDAC – Ireland
Sheffield University – UK

Edited Final Report

Executive Summary:

The edited final report covers all the work, objectives, results and conclusions for the entire project period from September 1st, 2002 - February 28th, 2005. Activities reported are in line with the project workplan as covered by the GEMSS Contract IST-2001-37153.

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1 Project Overview

GEMSS developed an interoperable, innovative Grid middleware for medical service applications building on common Grid standards. The focus is on innovative extensions that support medical applications including security models compliant with European legal issues, fail-over and recovery from errors as well as workflow and service orchestration techniques for time-critical processes. GEMSS is a two and a half year project which started in September 2002.

1.1 Objectives

The central objectives defined at the beginning of GEMSS project are to:

- demonstrate that the Grid can improve pre-operative planning and near real-time surgical support by providing access to advanced simulation and image-processing services,
- build middleware on existing/developing Grid technology standards to provide support for authorisation, workflow, security and Quality of Service aspects,
- develop, evaluate and validate a test-bed for the GEMSS system, including its deployment in the end-user's working environment,
- analyse and test the European Legal Framework from three approaches (Privacy, Contract, Liability) considering the use of Grid-based-technologies / applications partially provided through the Internet, in order to know if the European Legal Framework permits the development and the exploitation of such applications and if positive, under which constraints.

1.2 Main goals

The main goal of GEMSS was to provide end-users from the medical community with advanced tools at their workplace through easy-to-use interfaces. In particular GEMSS aimed at:

- the installation of a secure, extendible, interoperable and collaborative test bed for GRID-enabled medical application services,
- demonstrating the medical significance of the GEMSS models,
- demonstrating the functionality of the GRID-infrastructure,
- opening new business models for future commercial exploitation,
- analysing the main legal aspects to be considered when developing and implementing GRID-based technologies in the health area.

1.3 Priorities

Through the central objectives outlined in section 1.1 GEMSS was an infrastructure project driven by its 6 prototype medical service applications.

1.4 Main Results & Contact

The main results of the GEMSS project consist of an innovative middleware for the secure and lawful provision of simulation and medical image processing services and a set of medical application services all listed in the table below.

Table of main results at the end of the project
Middleware:
GEMSS Grid Middleware: A service oriented infrastructure for the secure and lawful provision of medical application services based on web service technology.
Services:
Maxillo-facial Surgery Planning Service: Grid-enabled interactive planning tool for maxillo-facial surgery.
Neuro-surgery Support Service: Grid-enabled quasi real-time neurosurgery support (prediction of the brain shift).
Monte-Carlo Radiosurgery Planning Service: Clinically useful Grid-enabled tool for validation of radiosurgery plans.
Inhaled Drug Delivery Simulation Service: Web-based, parametric simulation tool for the optimisation of inhaled drug delivery.
Cardiovascular System Simulation Service: Accessible cardiovascular simulation tool with sophisticated boundary condition support.
Medical Image Reconstruction Service: Grid-enabled advanced 3D image reconstruction.
Testbed:
The consortium decided to keep the testbed alive for at least one year after the end of the project. NEC will continue to operate its server to allow continued developments, support of services and pilot studies. This will support the post project exploitation activities.

After the end of project the GEMSS middleware is available as Open Source under the LGPL license from the download section of the GEMSS web site <http://www.gemss.de>

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1.5 Architecture

The GEMSS middleware is an implementation of a Service-Oriented Architecture based on standard Web services. Since GEMSS supports a public key infrastructure there can be a number of trusted certificate authorities to issue security certificates. Service registries hold details of where services can be found and are queried before a client interacts with specific service providers. Figures 1.1 and 1.2 show the client and server side of the Grid architecture. Deliverables D1.2a and D1.2b – Global System Design/Revision - have the full details.

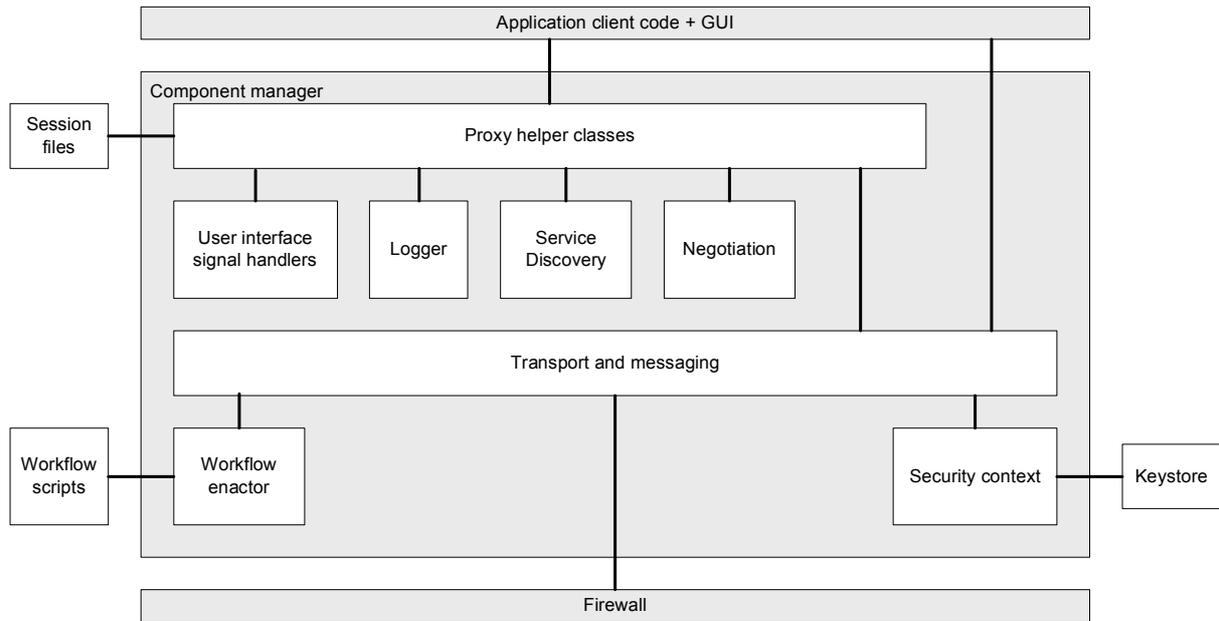


Figure 1.1: GEMSS client architecture

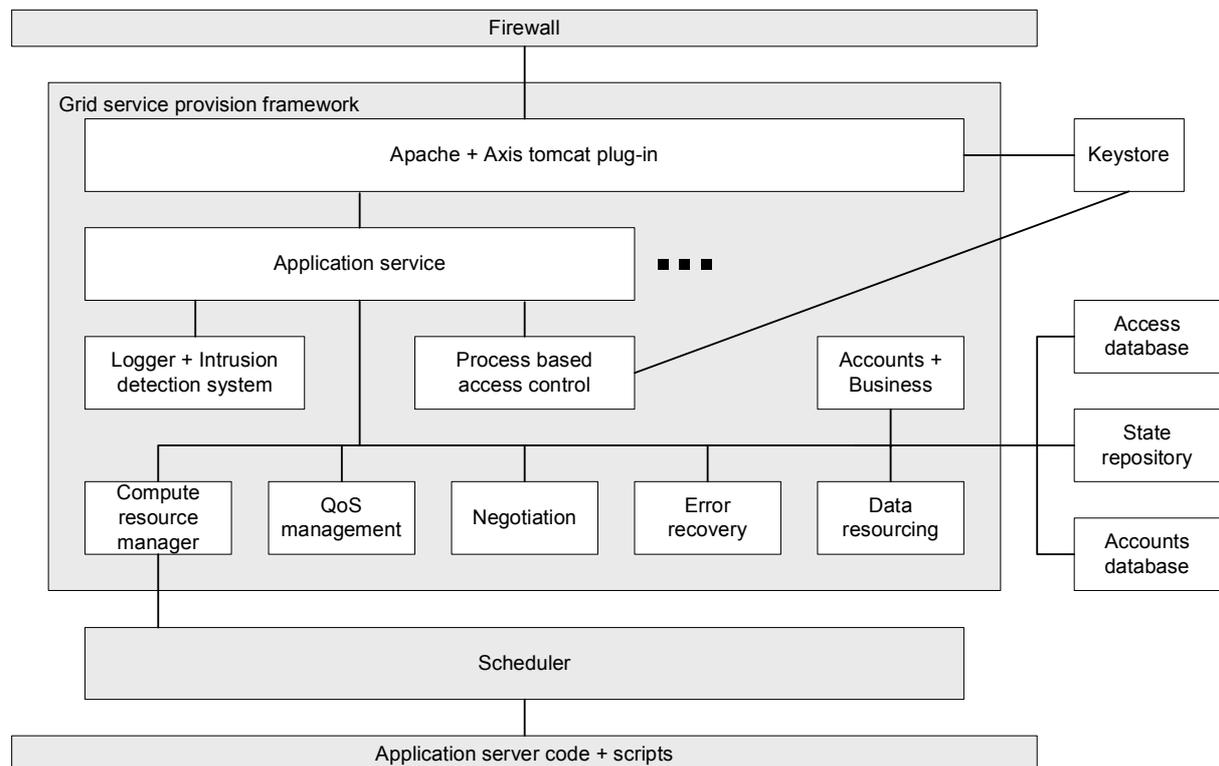


Figure 1.2: GEMSS server architecture

2 Consortium

The GEMSS Consortium consists of 10 partners, with three experienced in GRID technologies, two software developers, two University medical departments, and three end users, two of whom are specialist SME's in the area of bio-medical simulation. The Consortium thus represents a well balanced mixture of private and public partners whose activities range from basic research to industrial/commercial development and sales. The heterogeneous character of the Consortium has been designed to form a critical mass to best address the scientific requirements imposed by the problems to be solved.

No	Partner	Country	Specific Expertise, Role in the project
1	NEC (CCRLE)	UK	Finite element simulation, mesh generation, GRID-middleware, HPC software & hardware, Project Management.
2	MPI	Germany	Medical image processing, Model validation, Acquisition of scan-data, medical end-users.
3	ISS	Austria	Programming environments, software tools, HPC tools and hardware, GRID technology.
4	USFD	UK	FSI modelling, cardiovascular and respiratory applications. Provision of validation datasets, scan data. Clinical test site for radiosurgery application. Medical end user.
5	ANSYS (CFX)	UK	Software and applications.
6	IT-Innovation	UK	GRID technology and know-how, technology transfer.
7	CRID	Belgium	Consultant in legal issues
8	ASD	Germany	FE and CFD consultancy for artificial organs and biomedical devices.
9	IDAC	Ireland	Stress-analysis consultancy, Consultancy, ANSYS re-sellers, GUIs
10	IBMTP	Austria	Image reconstruction software, acquisition of scan data, clinical end users

The following table shows the involvement of partners in work packages. Work package and sub-task leaders are marked in red.

Partner	ST1.1	ST1.2	ST1.3	ST2.1	ST2.2	ST3.1	ST3.2	ST3.3	ST4.1	ST4.2	ST4.3	ST4.4	ST4.5	ST4.6	WP5	WP6
NEC	●	●	●	●	●	●	●	●	●						●	●
MPI	●		●						●	●					●	
ISS	●	●	●	●	●	●	●	●						●	●	
USFD	●		●								●	●	●		●	
ANSYS	●		●	●		●	●					●	●		●	
IT-Innov.	●	●	●	●	●		●				●				●	
CRID	●		●		●										●	
ASD	●		●									●	●		●	
IDAC	●		●	●		●	●	●					●		●	
IBMTP	●		●											●	●	

3 Progress Summary

3.1 Workpackage 1: System Design and Evaluation

This workpackage has three main responsibilities:

- to capture the system and end-user requirements,
- to produce a global design for GEMSS including the medical service applications and
- to evaluate the testbeds and the medical service applications within the testbeds produced during the course of this project.

3.1.1 Sub-task 1.1: Requirements Capture

The requirements capture process was performed in the first three months of the project and provided a sound basis from which to start the global system design. All partners were asked to list their requirements and these were refined into five categories. The five types of requirements are listed in table 3.1.

Type	Comments
Business requirements	Commercial requirements of the GEMSS business model both for the supplier and end-user of Grid computing power.
Legal and social requirements	Legal, and to a lesser extend social, requirements expected to arise from the availability of end-user medical services.
Security requirements	Security requirements of both medical end-users and suppliers.
Performance requirements	Performance requirements of end-user and suppliers.
Application requirements	End-user requirements for the medical services they wish to support.

Table 3.1: Requirement categories

Some of the most important requirements were found in the security category, since within GEMSS we are dealing with medical applications and must work with highly sensitive patient data. The security requirements were born in mind throughout the design of the GEMSS infrastructure, since from the legal analysis it was clear that we could not make patient data any less sensitive and had to ensure best practice security was applied throughout.

Deliverable D1.1 contains the full set of user requirements, and application use cases which formed the basis of the initial system design analysis.

3.1.2 Sub-task 1.2: System Design

The GEMSS middleware is an implementation of a Service-Oriented Architecture (SOA - see Fig. 3.1) based on Web services. Since GEMSS supports a public key infrastructure there can be a number of trusted certificate authorities to issue security certificates. Service registries hold details of where services can be found and are queried before a client interacts with specific service providers. Figure 3.1 shows the basic concept of the GEMSS SOA.

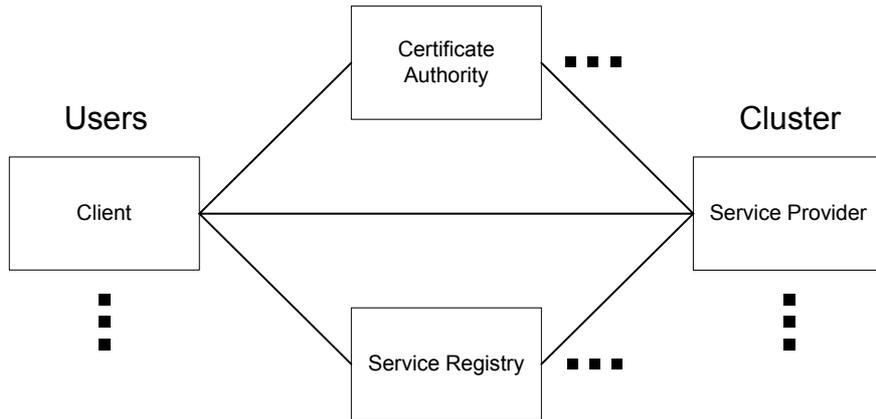


Figure 3.1: High-level GEMSS Service-Oriented Architecture

Client	Users who have a job to run.
Service provider	People who support the Grid servers that can run Grid jobs
Certificate authority	Third party who provides certificate authentication after appropriate identity checks.
Service registry	Registry holding a list of service providers and the services they support. Registries may be global or provided locally by a client.

Throughout the design that follows we have applied a three step process to job execution. First there is the initial business step, where accounts are opened and payment details fixed. The pricing model may also be chosen at this stage. Next there is a quality of service negotiation step, where a job's quality of service and price, if not subject to a fixed price model, is negotiated and agreed. Finally, once a contract is in place, the job itself can be submitted and executed. As discussed later, there is a hierarchical nature to these steps, with one or more quality of service negotiations expected per account, and one or more jobs per quality of service contract. Figure 3.2 illustrates this three-step process.

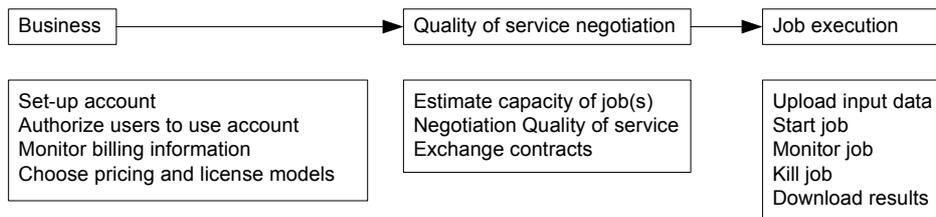


Figure 3.2: Three step process to using the GEMSS Grid

3.1.2.1 Client architecture

The client side of the GEMSS architecture is shown in Figure 3.3. The client would typically run an offline business workflow to open an account with a service provider and agree payment. When a Grid job is required to be run the client would then open negotiations with a set of service providers for a particular application job. The quality of service negotiation would then be run to request bids from all interested service providers who can run the clients jobs; this would result in a contract being agreed with a single service provider. The client would then upload the job input data, and any application workflow, to the service provider where the server side application would take over.

The component manager provides a way to dynamically load different versions of components as required, allowing flexibility of implementation. All components have a well-defined interface that the component manager knows.

Most workflow within GEMSS is encoded by the proxy helper classes and supports negotiation and job handling workflow. The client always drives the three-steps of the GEMSS process. The reason for this is the requirement to operate with firewalls and not tunnel holes through them. Given this, there can be no service provider initiated connections, or call-backs, to the client.

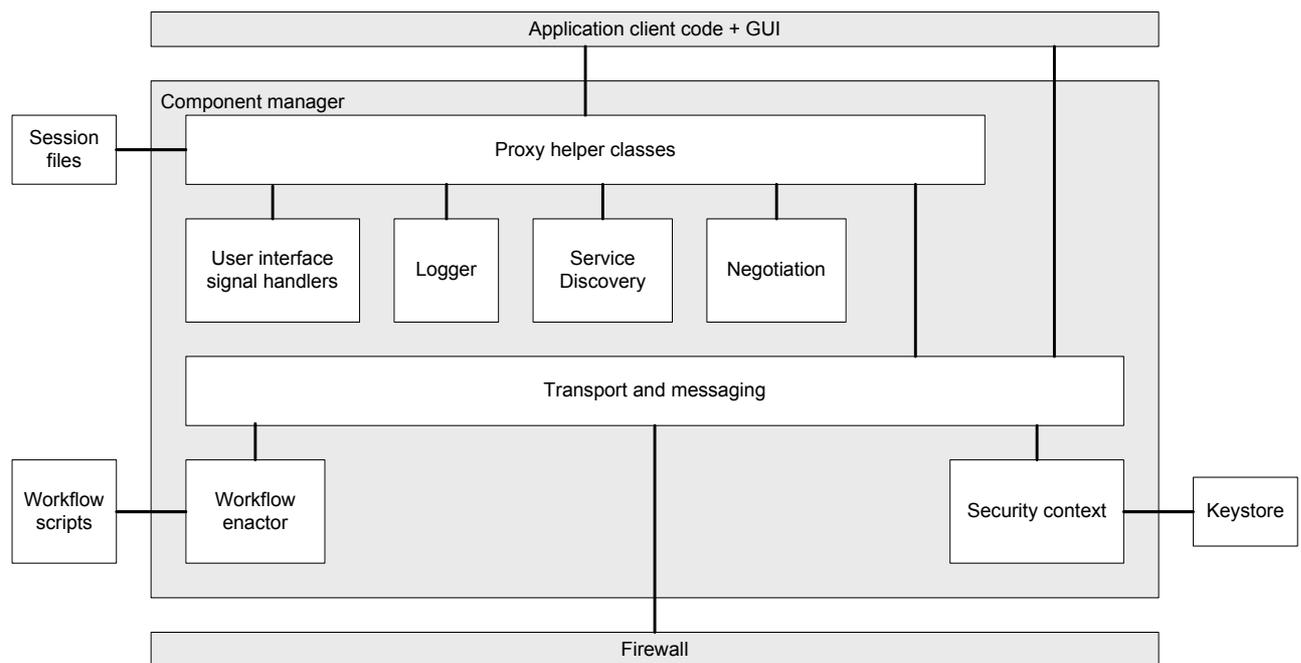


Figure 3.3: Client side of the GEMSS SOA

Application client code and graphical user interface

This is the application code, which is linked to the component manager. The application code provides a custom application user interface and manages the proxy helper classes. The major part of the client application code will be the user interface and job workflow orchestration.

Component manager

The component manager is a plug-in framework capable of supporting a set of components, each with well-defined interfaces. It provides a signalling mechanism that components can

use. Components in the component manager's code repository can be dynamically loaded as required by the application. The component manager also manages client sessions and provides a start-up and shutdown function the application can call when it is first run.

The component manager supports a mechanism to regularly check for patches to existing components and completely new components. This removes some of the burden on the users checking for upgrades, and could make fast security patching a practical feature of this system.

Logger

This is a low level logging component that is used by the service provider side intrusion detection system.

Negotiation

This component provides the functionality to run a client driven auction with several service providers. The result of this auction is an agreement to run a specific job. FIPA protocols are used to allow future agent support to the negotiation process.

Proxy helper classes

Proxy helper classes provide a simple interface that the applications can link to. These proxy classes are intended to be the main contact point for the applications, invoked via the component manager. There are proxy helper classes to run Grid jobs, agree quality of service details and negotiate with several service providers to get the best deal for a job. These proxies are persistent and support state, saved to session files, which allows jobs to be run over a protracted period without the need for a persistent client connection to the service provider.

Security context

This component supports maintenance of a security context. It provides a framework for generating, storing and verifying trust for security tokens of various types. It provides the security context used by the transport component for HTTPS and secure message encoding.

Service discovery

This component invokes the service registry and obtains a list of services that match a query. The registry this component searches can be specified by the client allowing only trusted service registries to be queried by the client.

Transport and messaging

This component is capable of creating low level messages, and sending them with appropriate transport bindings, as specified by the WSDL that defined the remote service. All calls to services are fed through the transport and messaging component. The appropriate WS security and WS policy procedures will be implemented before a message is sent, and before a response is passed to the other client-side modules.

User interface signal handlers

These signal handlers are a set of default handlers that applications can use. These signal handlers are only default handlers, and it is expected that a sophisticated application would create their own handlers, which would link directly to their own custom user interfaces.

Workflow enactment

This is a component capable of parsing and running a workflow language script. This component is expected to be used as a technology demonstrator for soft coded quality of service negotiation workflows.

3.1.2.2 Service provider architecture

The service provider side of the architecture is shown in Figure 3.4. Applications will be run by the service under the direction and orchestration of the client, subject to the necessary availability of and authority to use resources. The compute resources available at the service provider's site will be used to actually run the services. The quality of service management module is there to handle reservations with the compute resource job scheduler and provide input to the quality of service negotiation process so that sensible bids can be made to client job requests.

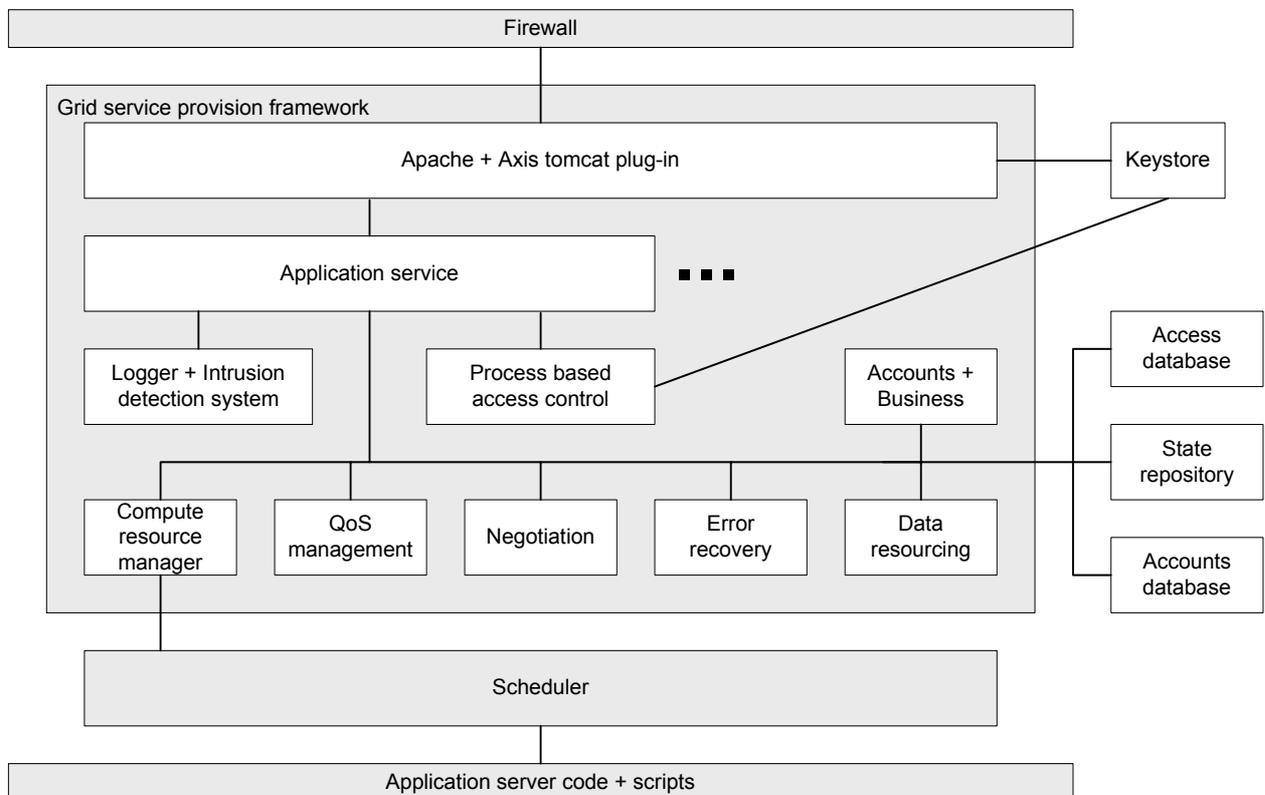


Figure 3.4: Service provider side of the GEMSS SOA

Accounts and business

This service maintains a database of auditable information about client accounts, including payment details and the current billing status. When jobs are run the business modules pricing models are used to calculate the payment due for resources used. A web interface is provided to allow client budget holders to access their billing status and review their account.

Application service(s)

The application service provides all the operations defined within the service WSDL file. These operations are routed to the appropriate module by various handlers, which are optionally installed at the service provider's site. The process based access control module is always consulted before an operation request is sent to a module.

Application server code and scripts

Each application must install its server side code and a set of scripts to run these codes. These scripts all have the same interface, and basically expect to receive an archived file containing the input data and produce a archived file with the output data. Start scripts invoke the scheduler as required by the service provider installation.

Apache + Axis tomcat plug-in

Tomcat plug-in's are used to support WS security enhancements. Tomcat itself provides the web service interface to individual application services whose functions are exposed via a WSDL interface.

Compute resource manager

This module is written to interface with the service provider's choice of scheduler. This module will be called to make reservations for jobs with the scheduler and start jobs. Since each service provider can have a different scheduler, along with different compute resources, there will have to be custom compute resource manager modules for each service provider.

Data resourcing

This module allows for persistent data between jobs, allowing intermediate files to be used as the input to other jobs etc. This is intended as a technology demonstrator within GEMSS.

Error recovery module

Closely linked to the compute resource manager, this module may use check-pointing to re-start or re-locate jobs as required (where the resource manager or the application itself enables this). This is intended as a technology demonstrator within GEMSS.

Grid service provision framework

This is a server side hosting environment that allows services to be installed and deployed.

Logger + Intrusion detection system

A module to securely log and analyse low level events in a distributed environment with the aim of detecting intrusion. The intrusion detection module may also integrate with

conventional non-grid intrusion detection subsystems associated with the web server. This is intended as a technology demonstrator within GEMSS.

Negotiation

This module provides server side support for a closed-bid reverse English auction. It supports FIPA protocols and calls the QoS management module to try to get the best reservation possible. Bids are returned to the client for interpretation by the client side negotiation component encoded as web service level agreements (WSLA).

Process based access control

This module maintains an access control database of allowed process actions. The application service and other server side modules will check with the process based access control module before any operations are invoked. This provides a mechanism to check the client's distinguished name, obtained from the WS security header information, and confirm the operation was expected and allowed.

QoS management

This module handles the QoS interactions with the scheduler, via the compute resource manager. The QoS management module takes a web service level agreement (WSLA) and tried to make a reservation with the scheduler to provide the required levels of quality of service. Initially temporary reservations are made until the client confirms the reservation and agrees to run the job.

The QoS management module required an application specific performance module from each of the applications that are installed for GEMSS. This performance module is used to estimate the exec time jobs will take given a metadata description of the jobs input data.

Scheduler

GEMSS assumes the availability of a service provider specific scheduler that supports reservation. We use NEC's COSY scheduler and the MAUI scheduler (LGPL license) within the project.

3.1.3 System Development

The final status of development work to date is shown in Figures 3.5a and 3.5b. The blue modules have been developed and the red modules are technology demonstrators. Technology demonstrator modules will not be released as part of the main software release, but will be worked on until the end of the project and form the basis of a proof of concept development.

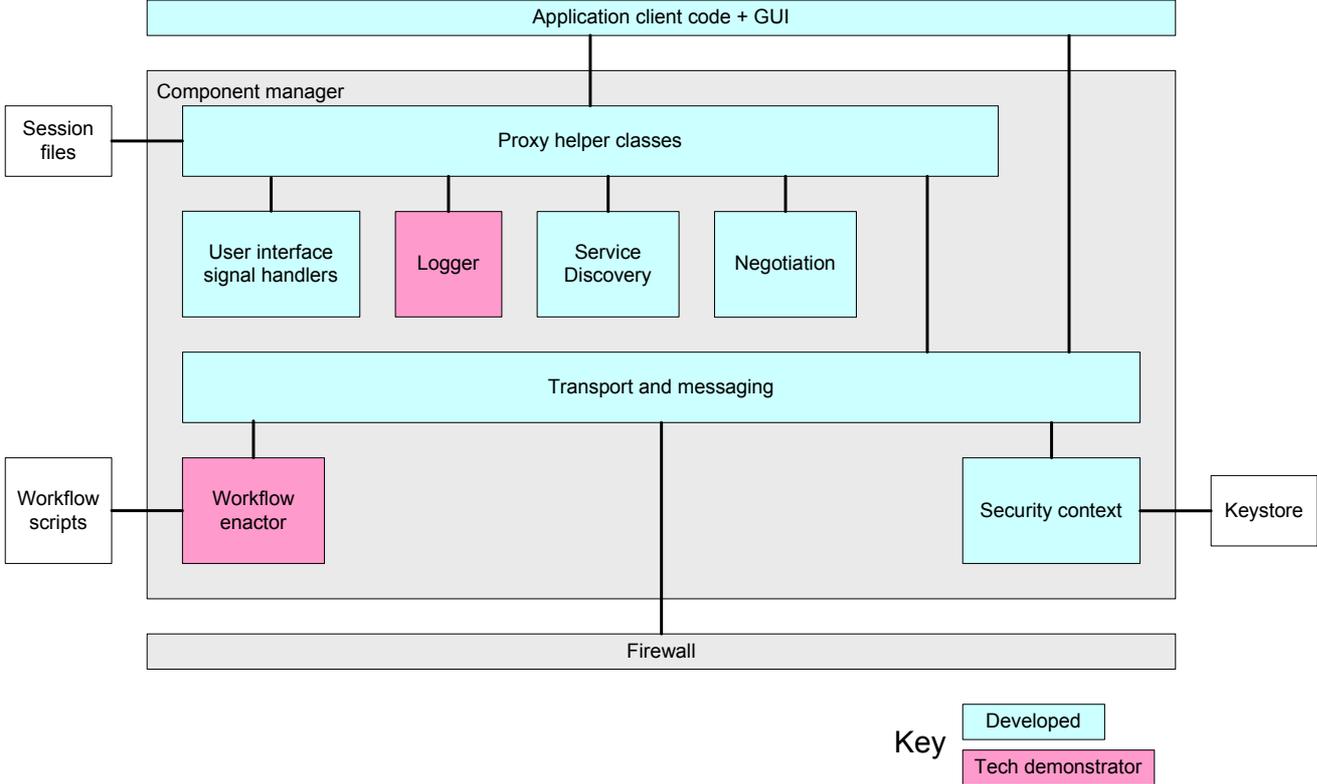


Figure 3.5a: Client module development summary.

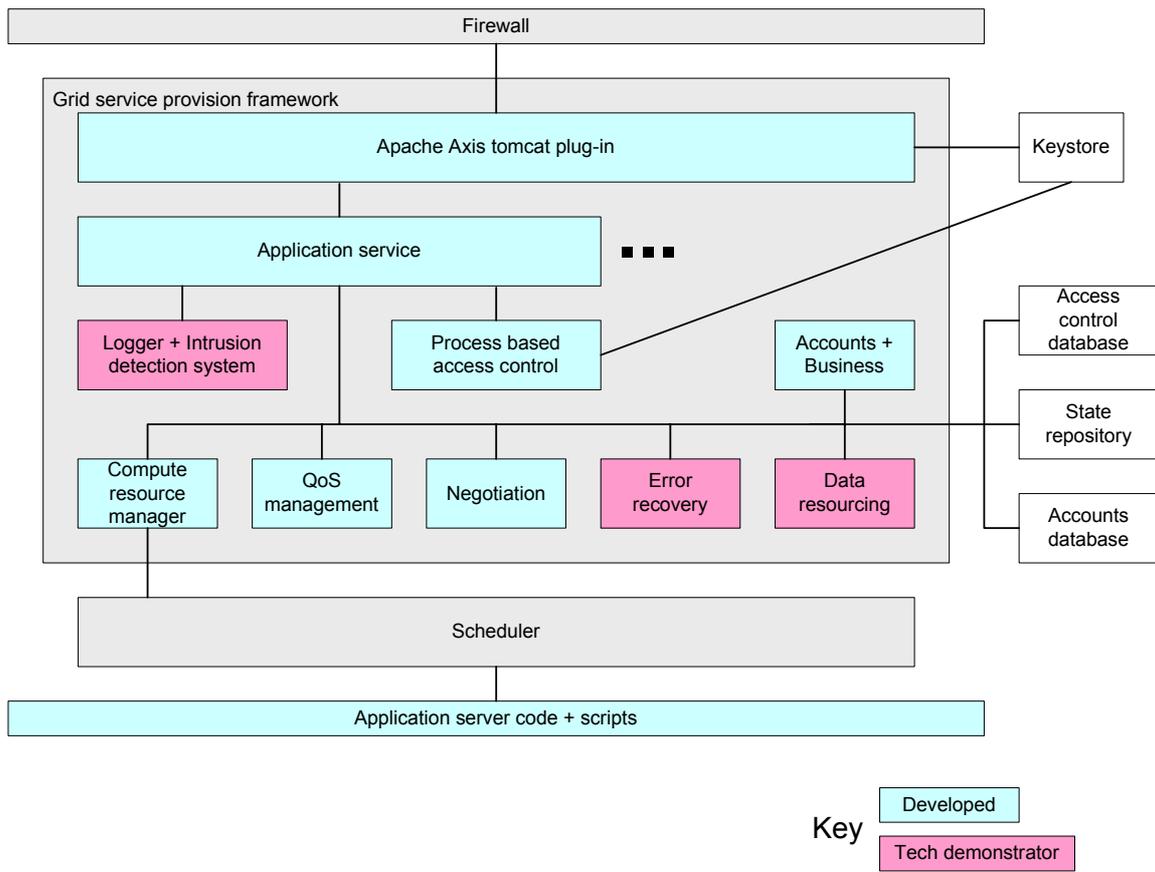


Figure 3.5b: Service provider module development summary.

Low-level details of each of these modules can be found in section 3.2 together with example sequence diagrams for common Grid activities.

3.1.4 Sub-task 1.3: Evaluation

At project midpoint, an evaluation of the software development progress was performed, and use case diagrams as well as system goals were re-evaluated. User and developer experience was collected in form of a questionnaire. All six medical applications are Grid-enabled, using the GEMSS middleware. Performance and robustness tests validated the various phases of the middleware design and demonstrated the quality of the implementation. This was documented at midterm in deliverable D1.3a.

Four tests were performed as part of the mid-term evaluation:

- The infrastructure test assessed the file transfer delays, showing how the size of the data set and the hardware use effect performance.
- The application testing characterized each application in terms of how it reacted to more CPU's, revealing some of the differences in nature between each of the six GEMSS applications.
- A 19 hour robustness test was conducted with all six applications, showing the GEMSS infrastructure to have excellent robustness when running jobs over the unreliable Internet.
- Two of our applications performance models were assessed, providing an early insight into this work which is actually planned for after the mid-term release.

Important feedback was given by the application developers to optimise and level out a few problems regarding the middleware:

- The certification process and Java keystore setup should be optimised.
- The interaction of the scheduler and the GEMSS server system is an issue.
- Some of the design goals were re-prioritised during the Namur meeting in February, 2004, in order to better match requests and remaining development effort.

This final evaluation report D1.3b includes an evaluation of the final GEMSS system, a survey regarding the application developer experience, and a test of the performance of the GEMSS system.

The results of the evaluation can be summarised as follows:

- All six medical applications are now Grid-enabled, using the final phase I3 version of the GEMSS middleware. Some of the applications are already ported to the phase I4 technology demonstrator.
- Multiple stress tests were conducted to burden the middleware with a high load sufficient to break it, with tests lasting from a couple of days to a whole week. These tests revealed bugs within the server side parts of the middleware and after fixing, performance and robustness tests validated the middleware design and demonstrated the quality of the infrastructure.

- A long term test of the middleware provided information about the standard usage of the GEMSS middleware, lasting several months. Negotiation and file transfer overhead were measured and showed that the middleware is most suited for applications with a relatively long run-time. This is consistent with the testbed applications implemented by the GEMSS consortium since they normally require such long runtimes.

Important feedback from the application developers allowed the identification of a few obstacles regarding the exploitation of the middleware:

- The certification process and Java keystore setup could be optimised further.
- The Client installation of the middleware could be supported by a cross-platform GUI installer in order to hide the complexity of the installation process.
- A server side standardisation of the execution environment would facilitate the integration and deployment of the application services at different service providers.
- A tutorial describing the steps necessary to port a high performance application to the GEMSS infrastructure could be part of the final release.

The final evaluation task was to deploy the client software at medical end user sites and gather their feedback about the usability and usefulness of the tools resulting in a project internal report (D1.3c) at the end of February 2005.

3.2 Workpackage 2: Grid Services & Security

3.2.1 Sub-task 2.1: Workflow and Quality of Service

3.2.1.1 Quality of Service

Quality of Service is a crucial issue in the context of providing medical applications on the Grid. The GEMSS infrastructure aims to provide application level Quality of Service by explicit timeliness guarantees for the execution of medical applications on a case by case basis, as well as implicit Quality of Service of the middleware (e.g. highest level of security – best practise). All explicitly formulated QoS guarantees such as execution time and price are agreed between a service consumer and a service provider in form of an XML document following the Web Service Level Agreement (WSLA) specification.

Design

The GEMSS QoS design comprises the registry service and discovery component, the QoS negotiation subsystem, the QoS management subsystem, and the error recovery subsystem. The QoS negotiation subsystem, which handles the negotiation process, comprises a client component (advanced QoS negotiation component) and a service module (QoS negotiation module). The QoS management subsystem shown in Fig. 3.6 includes the management of QoS requests and offers by interacting with the compute resource management to ensure advance reservation of resources (e.g. CPU time). Advance reservations are based on estimates provided by the application performance models. Furthermore, the QoS management monitors the progress of submitted jobs via the compute resource manager. The error recovery module handles check-pointing and re-starting or re-allocation of jobs. Check-pointing/restarting must be supported by the scheduling system and/or the native application.

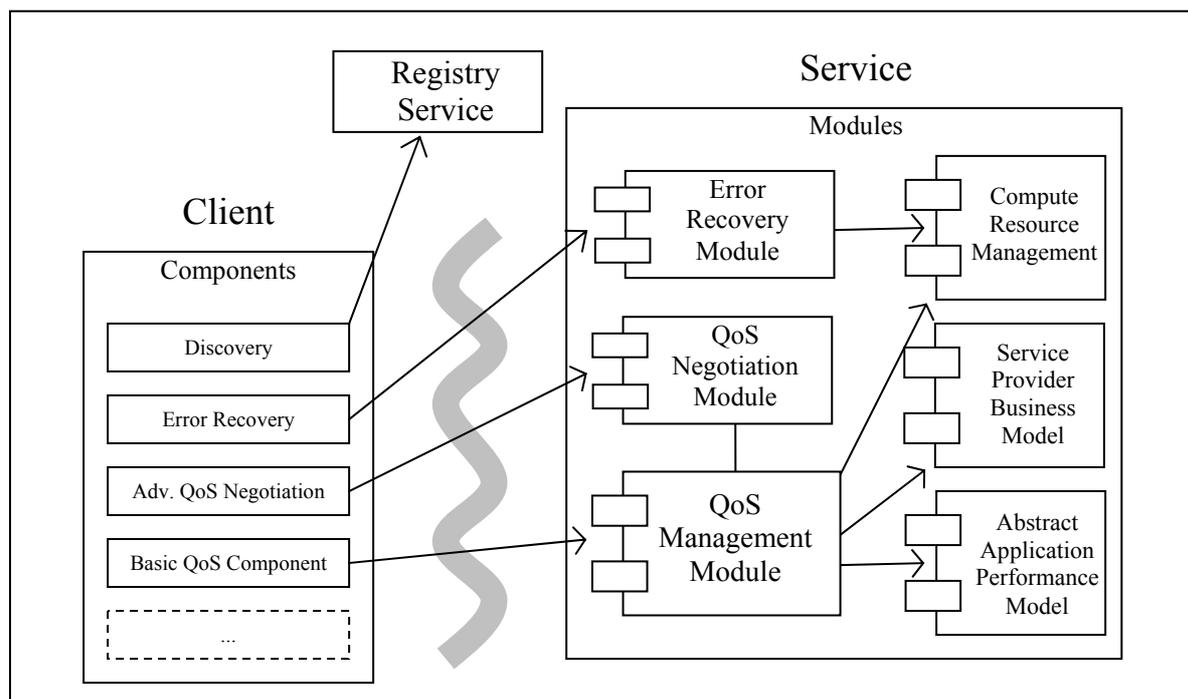


Figure 3.6: Quality of Service related components in the GEMSS framework.

Service registry

The GEMSS Service registry has been designed as standalone web service that provides operations for service (un-)registration and advanced service query. Each service provider maintains a service registry that contains all installed services hosted by the service provider. The service registry contains all information about a registered service available at the time of installation. The information about services stored in the registry comprises common attributes (service category, service endpoint URI, etc.) and specific attributes which are arbitrary name-value pairs. The query mechanism also supports queries with both common and specific attributes.

As standalone web service the GEMSS Registry Service is component-independent, i.e. it has no dependence on the other GEMSS components/modules and it can be used within standard web services hosting environment (e.g. Apache Tomcat).

A GEMSS registry V1.0 following the specification has been released. It contains a standalone web service that may be installed within the GEMSS hosting environment. Additionally a command line tool is provided in order to support registration and unregistration of services. This tool is also used within the GEMSS service provision framework in order to publish installed services in the GEMSS registry service.

Service discovery

The GEMSS Service discovery component has been designed and released as a client component fitting in the GEMSS client pluggable component framework. The discovery component provides advanced service discovery by querying remote GEMSS registry services. A client application or any other GEMSS client component may use the discovery component in order to discover appropriate services within a given set of registry services. The discovery component provides an abstract API allowing potentially multiple implementations of the service discovery component to be provided. The connections between service and registry are secured using web service and transport security.

QoS XML-message exchange

The message exchange in the GEMSS QoS system is based on XML documents. A client describes a request by providing an XML Request Descriptor which contains meta-information about the request (e.g. mesh size, number of iterations, etc). For the QoS requests and offers processed by the QoS management, initially the following documents are used:

- QoS Descriptor: Describing agreed QoS properties between service provider and consumer
- Request Descriptor: Describing application specific meta information about the client request
- Performance Descriptor: Describing the output of the application performance models like estimated runtime, memory requirements, etc.

The WSLA (Web Service Level Agreement) specification was evaluated and incorporated in order to perform QoS negotiations in a standard format. Thus, QoS contracts and descriptors follow the WSLA specification.

Advanced Quality of service negotiation

The GEMSS quality of service negotiation involves a single client negotiating with one or more service providers, each of which is competing to win the client's business. As negotiation strategy a "closed-bid reverse English auction" protocol was implemented. This

auction protocol has been examined in the Agent research area and is encoded within the FIPA agent communication standards.

The GEMSS negotiation code automates the service discovery steps and auction protocol. The underlying mechanism for both discovery and negotiation is thus hidden from the user via a simple interface. This interface can be used via the GEMSS pluggable client component framework.

Basic Quality of Service Negotiation

Besides relying on automated QoS negotiation (reverse English auction), arbitrary negotiation strategies may be implemented manually using directly the methods provided by the basic QoS negotiation component, which provides a client-side API for the QoS negotiation. The GEMSS basic QoS component has been designed and released as a client component fitting in the GEMSS client pluggable component framework

Performance Estimation

A crucial aspect of the GEMSS QoS infrastructure is performance estimation. GEMSS relies on application specific performance models which are to be provided for each GEMSS application. Each performance model may be implemented differently depending on the nature of the application. Within GEMSS performance model implementations have been designed and implemented for all six applications as well as tested on at least one Grid Site.

Compute Resource Manager

The GEMSS QoS Infrastructure requires a scheduling system that supports advance reservation. Therefore the COSY scheduler developed by NEC has been successfully integrated via an abstract interface and is used to handle advance reservation of HPC resources. Furthermore an adapter for the the MAUI scheduling system to implement the generic GEMSS compute resource manager interface has been developed and integrated to proof independence of the QoS system from a concrete scheduling system.

Error Recovery

The Error Recovery subsystem has been designed as technology demonstrator for GEMSS. The Error Recovery supports up- and downloads of check-pointing data as well as restarts of applications if supported by the native application and/or the scheduling system.

3.2.1.2 Workflow

Design:

There are three levels of workflow in GEMSS, job handling, quality of service negotiation and business workflow. These features have been introduced as hard-coded workflows, and towards the end of the project the negotiation workflow has been examined for soft-coding as a technology demonstrator.

Soft-coding workflow is useful since it allows different service providers to perform negotiation, business processes, job handling etc differently without the client having to know. The client would simply download a service provider's workflow for a specific service, or set of services, and enact it. Potentially this will make the problem of adding new services and service providers to the Grid much more scalable, and reduce the integration time involved in using services.

Initial hard-coded workflow:

The initial workflow has been hardcoded in the phase 3 & phase 4 prototypes, with job handling and negotiation workflow encoded into proxy components. Full details of the proxy components are available in the design deliverable D1.2b.

The GEMSSProxy provides an easy to use Java interface representing the GEMSS application service. As a proxy it provides java method wrappers for each of the application services functions, hiding the transport component invocation calls that are required behind the scenes. The GEMSSProxy component thus provides everything the application developers need to run jobs.

The GEMSSNegotiator provides all the functionality of the GEMSSProxy, but with additional support for negotiation workflow. This class will automatically conduct an auction with a number of service providers and agree the best WSLA contract with one of them.

Shipped with the phase 3 & phase 4 prototypes is an example application that demonstrates how to use the proxy classes and run Grid jobs. The workflow to run GEMSS jobs is pretty simple, whilst the negotiation workflow is more complex. The full workflow can be seen in figure 3.7. An interface screen shot is shown in figure 3.8 of the sample application's GUI "in action", processing this workflow.

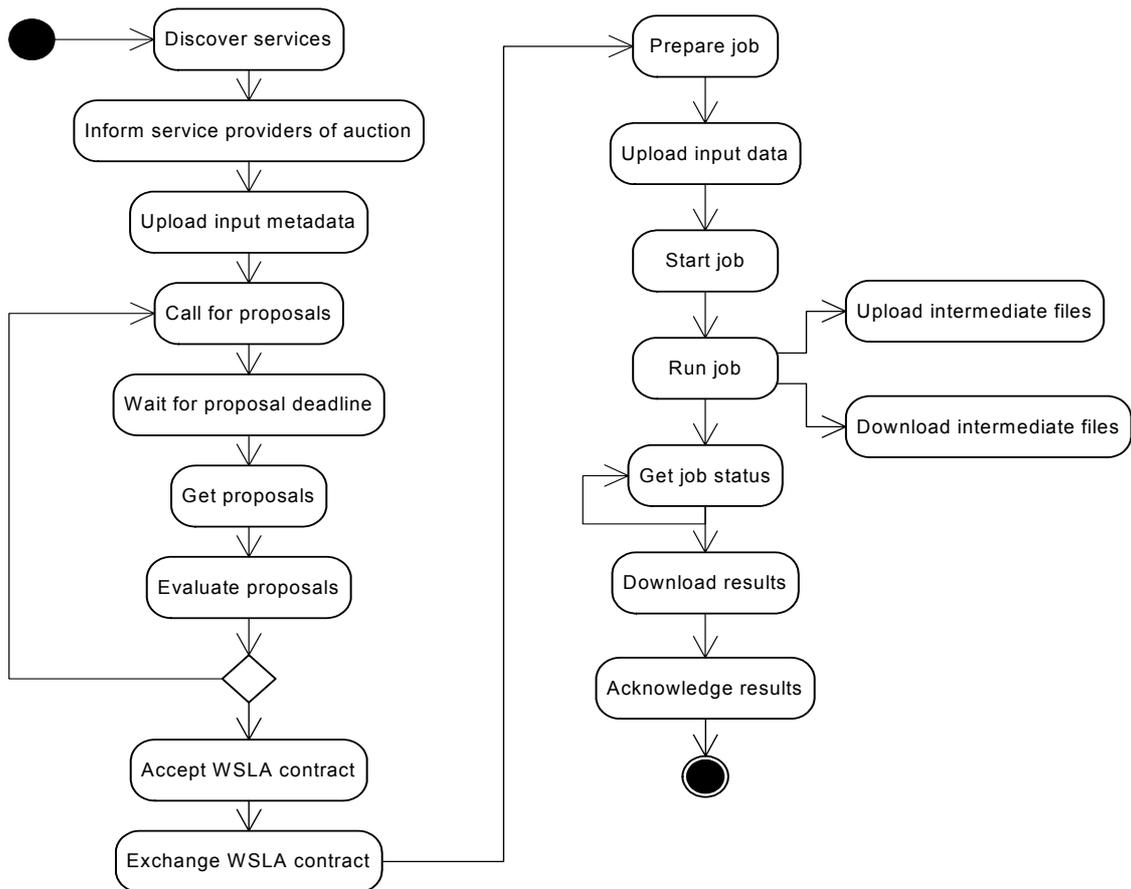


Figure 3.7: GEMSS workflow

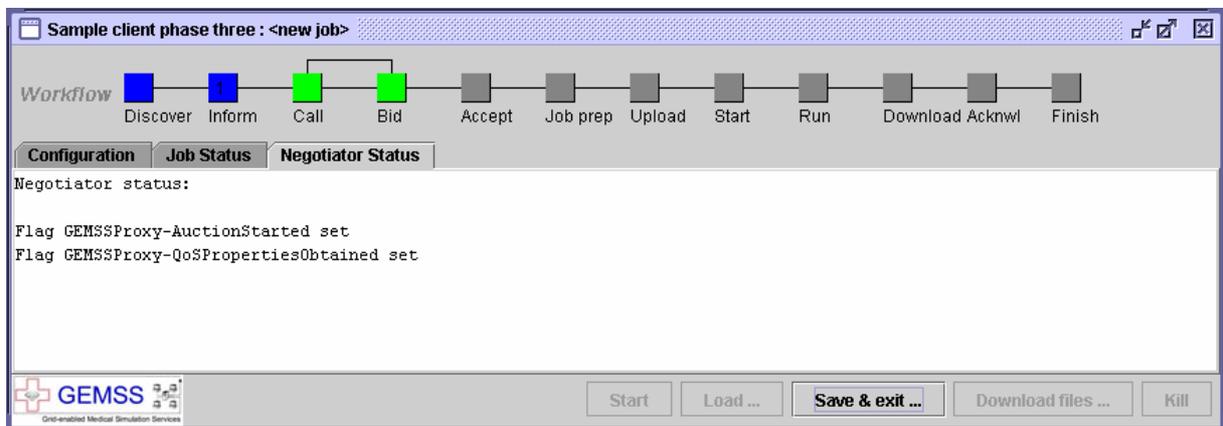


Figure 3.8: Screen shot of the example application shipped with the phase 4 prototype

The GEMSSNegotiator is a helper class that has, as an attribute, a GEMSSProxy instance. The purpose of the GEMSSNegotiator is to hardcode the quality of service negotiation workflow, allowing all negotiation steps to be performed automatically. The application using a GEMSS Negotiator component need not worry about either service discovery or negotiation with different service providers for the best deal.

Evaluation of the FreeFluo workflow enactor and ScufI workflow language:

The ScufI language: This section contains a short summary, based on the work being performed in the myGrid project [3]. The ScufI language is a high-level conceptual workflow

language and full details of Scufl can be found on the Taverna Open Source project site <http://taverna.sourceforge.net>. Commercial workflow enactors and languages exist, such as IBM's BPEL4WS, but within GEMSS we have restricted ourselves to the promising workflow enactor called FreeFluo, which has been released as LGPL. FreeFluo enacts the Scuf workflow language, and a Scuf definition consists of three main entities.

Processors: A processor can be regarded as a function of some set of input data to a set of output data, where each function may have side effects on the execution environment that are not encapsulated within the input / output specification. Processors have a set of named input ports, a set of named output ports, a name within the scufl space, and a current execution status (initializing, waiting, running, or completed).

Data links: A data link represents the consumption of some processor output by an input of some other processor. In fact, there is nothing in the language to prevent a processor consuming one of its own outputs, although this may be rejected during the translation to some other format due to the implicit problems with cyclic workflows. Data links have a source processor and output port name, a sink processor and an input port name and an optional name within Scuf space.

Concurrency constraint: Although the data link specifications are enough to ensure correct execution ordering, since processors are allowed to have side effects on their environment it is often required to explicitly create constraints on the ordering of execution of different processors. It is possible to create a gate constraint that must be satisfied before a processor can effect a particular state change; for example, processor one is only allowed to shift state from waiting to running when processor two has status 'completed'. Constraints have a processor controlled by the constraint, a state change blocked in that processor, a gate condition, and an optional name within scufl space. Concurrency constraints are particularly useful in dealing with stateful interaction with services as shown below.

The FreeFluo workflow enactment engine: Freefluo is a Java workflow orchestration tool for web services that currently supports a subset of WSFL as well as Scuf. Freefluo is very flexible and at its core is a reusable orchestration framework that is not tied to any workflow language or execution architecture. The enactor core supports an object model of a workflow in the form of a directed graph where each node has a state machine that defines its lifecycle. Workflow scheduling and state transitions are driven by message passing between nodes as execution of the workflow progresses. The core of the enactor is decoupled from both the textual form of a workflow specification and the details of service invocation and the data model. This allows the core to orchestrate a workflow in a generic way.

The enactor core is used in the context of a particular language and service run-time environment. A workflow language parser is used to convert a textual workflow specification, e.g. a Scuf document, into the internal object representation of the enactor core. An invocation framework is then added to allow the enactor to actually invoke services in the run-time environment and deal with the specific data types passed between the services invoked, e.g. WSDL calls and XML message parts.

Freefluo can easily be extended to support different invocation methods (Web Services, Grid Services, CORBA) and has been used in other projects in this way, for example for using CORBA wrapped numerical methods and data sets in a steel modelling workbench currently in use by the European Coal and Steel Community. Details of the Freefluo Open Source project site can be found at <http://freefluo.sourceforge.net>.

It is the ability to extend the enactor's run-time that also enables easy integration of stateful services, since the 'mini-workflow' of using these services can be encapsulated in bespoke extension. Furthermore, the run-time extensions are a natural and simple place to provide features such as iteration over datasets and automatic type casting or conversion.

Freefluo also supports generation of provenance information (what, when and where for all activities performed in a workflow) and also provides service discovery via standard UDDI if a service is not bound in a workflow specification (soon to be supported in ScufI).

An example ScufI workflow, created using the Taverna workflow-authoring tool, is shown in figure 3.9. The ScufI specification describes how to orchestrate the set of Web Services that provide the required functionality. The triangles at the top of Fig 3.9 are workflow inputs, the triangles at the bottom are workflow outputs and the green ovals are Web Service operations. The solid lines represent the data flows with the text annotations showing the data types.

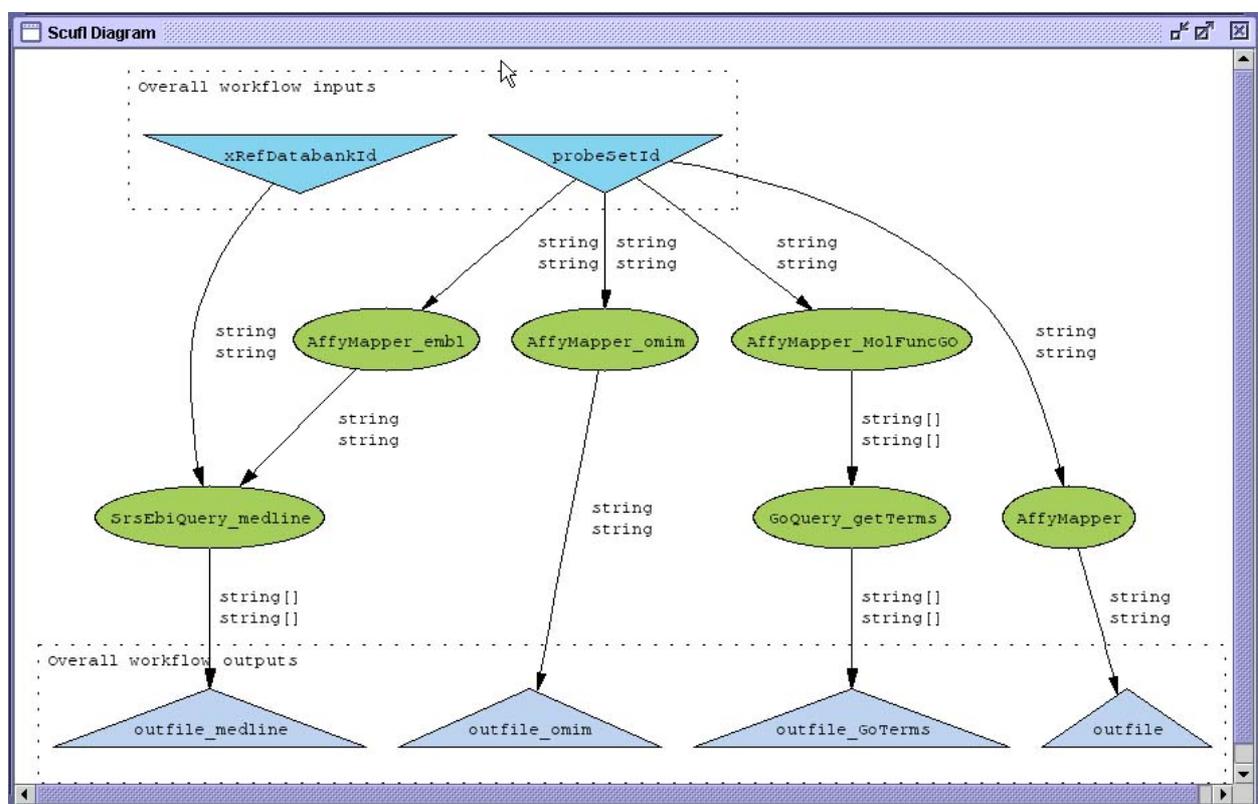


Figure 3.9: Taverna workflow-authoring tool

ScufI can also reference multiple types of workflow, such as in figure 3.10. Here some parts of the workflow require the use of two applications. Services are colour coded according to type, and the important thing to note is that these all appear at the same level of abstraction to the user despite the different levels of complexity of invoking the Web Services involved. Also shown in the diagram is a series of Web Service invocations that are cascaded together using control links. This set of invocations corresponds to the use of a stateful Web Service where a series of calls needs to be made in order to execute the application and retrieve the results. In this case, the series of invocations is explicitly visible to the user, as they are not abstracted through an extension to the workflow enactor. It should be clear from this example how the workbench and enactor could be used to invoke other stateful applications, e.g. using CORBA or Grid Services.

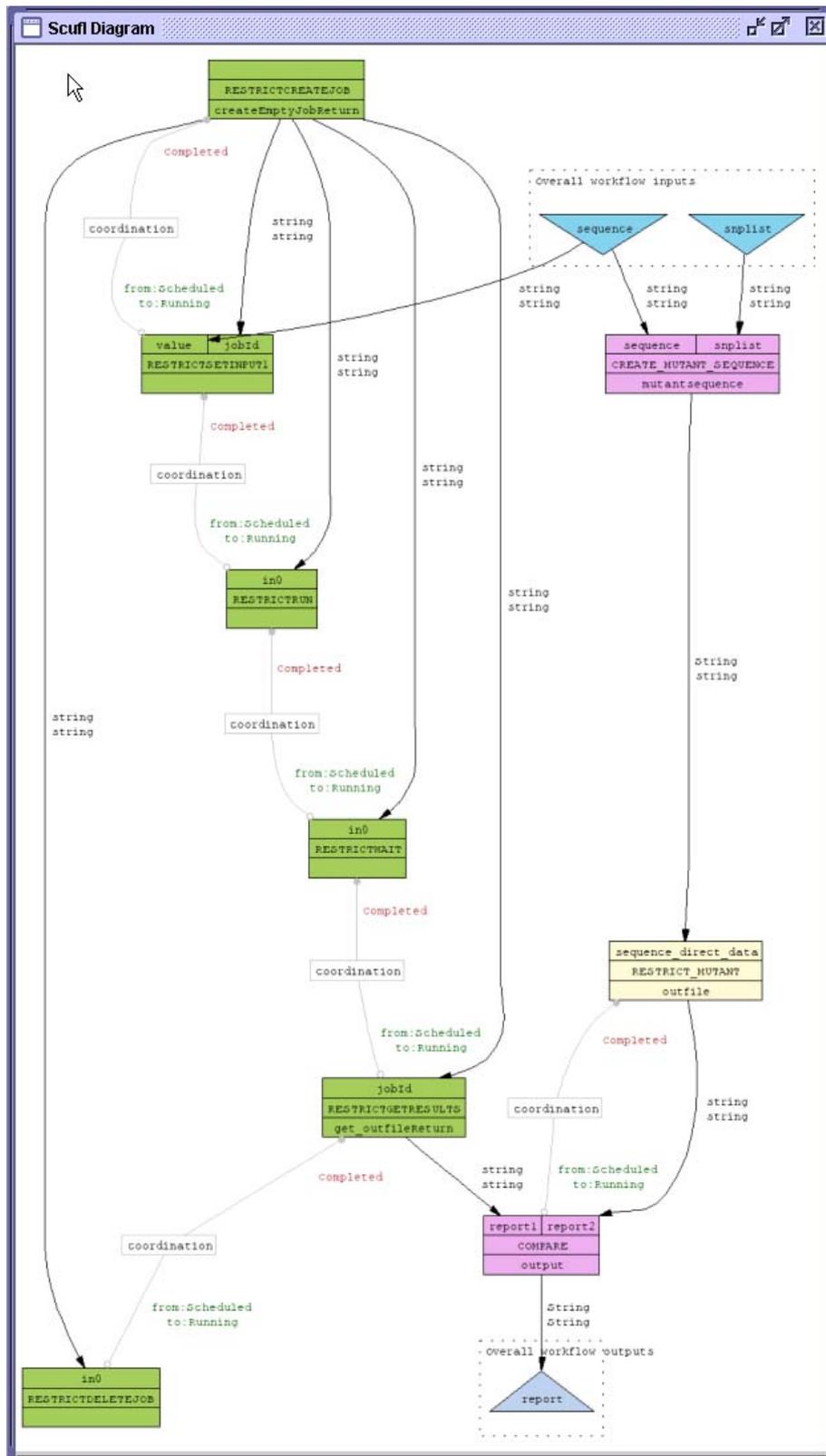


Figure 3.10: Incorporation of different types of services into a workflow

We feel that FreeFluo offers excellent opportunities for GEMSS, and could easily be wrapped up as a client side GEMSS component. Since the FreeFluo code has been released as LGPL there are no licensing issues, and since IT Innovation created FreeFluo as part of the myGrid project they already have in-house expertise in using this tool.

3.2.2 Sub-task 2.2: Security and Legal Issues

3.2.2.1 SECURITY ISSUES

3.2.2.1.1 Security assessment methodology

The first task performed was to create a security methodology for GEMSS, which users of the GEMSS infrastructure could apply to assess their own security. Security is like a chain, and a chain is only as strong as its weakest link. As such the security assessment methodology aims to enable users to examine their own security weaknesses, and thus enable them to address issues and improve the security of the overall GEMSS Grid. Deliverable D2.2a – Report on Methodology for Assessing Security - contains this methodology.

An asset-based analysis was proposed, which should be used to assess cost-benefits and effectiveness of GEMSS grid security features. To take account of the special properties of grid systems, the analysis should encompass dependencies on external assets, and others dependencies on one's own assets.

The main threats identified for a health Grid are:

- *Skilled crackers*: Skilled people who attack systems out of a sense of challenge. They typically do not have huge resources but do have plenty of time and the ability to find and exploit new and previously unexpected weaknesses.
- *Script kiddies*: Medium skill crackers that use the tools created by skilled crackers to perform exploits. As such they can only attack old weaknesses that will normally have patches available. However, not all system managers keep security patches up-to-date so these attacks are frequently successful.
- *Criminals*: Crackers who are motivated by financial reward for their exploits. They will use hacking tools to exploit weaknesses that will return financial reward.
- *Malicious insiders*: Disgruntled employees who have an axe to grind. They typically will have a high level of access and be very familiar with the operation of the Grid.
- *Incompetent insiders*: Users who unintentionally compromise security by failing to protect security-critical assets (e.g. passwords and private keys) or by foolishly importing malicious software or data.
- *Zealous commercial interests*: We expect that health-related grids will eventually involve not just clinicians and medical researchers, but also interested companies such as health insurers and some large employers. These companies can gain significant business benefits from access to grid-based data about (say) patients or competitors. Over-zealous attempts to access this data, potentially including clandestine industrial espionage, should be considered.

Given these likely threats, the most likely attack modes are:

- Social engineering attacks including impersonation, repeat fault attacks, etc.
- Brute-force cryptographic attacks against password files and private keys, if they can be obtained.

- Authentication attacks, including falsification of identity (by malicious insiders), and man-in-the-middle attacks.
- Authorisation escalation attempts including exploitation of bugs in services and very frequent scripted attacks.
- Network attacks including denial of service and distributed denial of service, and traffic spoofing possibly in combination with domain name service attacks.
- Malicious software including Trojan horses and viruses (that may be accidentally imported by insiders or deliberately planted), worms and root kits.

Because GEMSS is working with a health Grid, where patient data is being used for computation, the damages expected from security breaches are substantial. Litigation in the region of millions of pounds could well be expected if patient data is negligently handled.

It was suggested that the following defence options be seriously investigated for use in GEMSS, since they appear both cost effective and do not impose a large performance penalty. An analysis is of course be needed for each partner site to make an accurate appraisal.

- Encryption methods and secure communication protocols should be widely employed to authenticate communications and data and protect them from unauthorised access (this is standard practice on any grid).
- Access controls should be implemented as a matter of course.
- Software security should be implemented where necessary – e.g. to contain compromised processes or reduce the risk of importing trojans or viruses.
- Network security should be employed – firewalls are now more-or-less standard, but other techniques may be needed to counter some threats. A critical aspect of grid network security is to ensure it is consistent with existing measures against conventional threats.
- Security in depth should be maintained including standard practices such as logging. Measures such as intrusion detection and security audits should also be considered. The design of GEMSS should take account of the need for security updates, etc.
- The legal and policy issues should also be addressed. In the limit, one must have some sanction if one manages to catch an intruder, even if they are a legitimate grid user acting in accordance with the law in (over-zealous) pursuit of legitimate interests.

The outcome of the analysis of assets, threats and defences should be an estimate of:

- i) the annual financial cost of establishing and maintaining security defences (should be affordable);
- ii) the expected annual cost of attacks thereby prevented (should be greater than the cost of defences);
- iii) the expected annual risk and cost of attacks not prevented (should be acceptably small).

What is an affordable defence or an acceptable risk should be determined by comparison with the cost of defences and the level of risk present without using the grid. The incremental cost and risk of grid participation should be small.

The analysis of GEMSS security has been carried out by each participating organisation. The overall infrastructure was the same for all, but the costs and benefits of some local measures may be different for each participant. The goal was to enable each GEMSS partner to use the grid without excessive cost, while maintaining acceptable security for other users.

3.2.2.1.2 Security review

The security review has been published in deliverable D2.2c and did the following:

- Summarised the requirements for any GEMSS security infrastructure system
- Introduced an assessment methodology for evaluating technologies and toolkits
- Introduced and assessed possible enabling technologies and standards for providing the functionality defined by the requirements
- Established what constitutes best practice in terms of authentication, authorisation, accounting, data privacy
- Reviewed possible Grid solutions
- Evaluated off-the-shelf implementations of best practice technologies and standards.

The GEMSS security model is composed of a mixture of traditional security measures and new service-orientated security. Toolkit and technology choices for each part of the security model are based on best practice techniques.

The proposed security model has been implemented over the course of the project. The implementation plan reflects the dependencies between parts of the security model and dependencies on components within the global system design. Components that are implemented within GEMSS are not described in detail because they are described in 'GEMSS Global System Design' however these components will be developed using the best practice standards and toolkits established by this report.

Security model implementation included the following parts:

1. GEMSS PKI – Established GEMSS public key infrastructure including CA and RA representatives for each consortium partner.
2. Security Context Module – Developed security module that enables access to basic PKI authentication mechanisms deployed at Grid sites.
3. Transport and Messaging Module – Developed module capable of making HTTPS connections to services and encoding WS-Security integrity information.
4. Enhanced Security Module – Developed a module that extends and coordinates both the Security Context Module and parts of the Transport and Messaging Module in

order to provide for end-to-end mutual authentication, key-exchange and message confidentiality in situations where a Grid site that is composed of more than one security domain.

5. Apache-based Grid server – Provided mechanisms to host GEMSS services behind Apache SSL server.
6. Logger Module – Developed module for systematic logging of GEMSS events and data processing. The logging module will collect and log events at various points in the GEMSS system. The logging module forms the basis of the intrusion detection system.
7. Intrusion Detection Module– Developed module for detecting malicious use of GEMSS software.
8. Security Response Infrastructure – Developed basic response process for all sites including security advisory service.
9. Conversational Authorisation Module – Integrated GRIA process-based authorisation into GEMSS server side infrastructure.

3.2.2.2 LEGAL ISSUES

The European Privacy Legal Framework has been analysed considering the development and the exploitation of the six specific applications of the GEMSS project. The main result is that these applications may be developed and exploited under certain conditions.

3.2.2.2.1 Privacy approach

- Using GEMSS applications implies processing of personal data concerning the patient's health. The health practitioner will collect and dispatch the patient's personal data (e.g. imaging) through the Internet to the GEMSS provider.

The GEMSS provider will process (alone or with the support from other subcontractors) the patient's personal data in order to complete the therapeutic purpose of the data processing or the scientific research, before sending back the processed data or making them available to the health practitioner, again through the Internet.

The issue of data processing where using the GEMSS applications is only one aspect of the processing of patient's personal data concerning health by his/her health practitioner for therapeutic purposes and for scientific research.

- Many rules issued from different authorities concern the protection of privacy where processing patient's personal data and medical data by his/her health practitioner for therapeutic purpose and scientific research, such as :

- Article 8 of the European Convention on Human Rights and the judgements of the European Court of Human Rights,
- Article 7 & 8 of the Charter of Fundamental Rights of the European Union, the Convention of the Council of Europe for the protection of individuals with regard to automatic processing of personal data,
- Recommendation (97) 5 of the Council of Europe on the protection of medical data,
- Recommendation (83) 10 of the Council of Europe on the protection of personal data used for scientific research and statistics,
- Directive 95/46 on the protection of individuals with regard to the processing of personal data and on the free movement of such data,
- Directive 2002/58 concerning the processing of personal data and the protection of privacy in the electronic communications sector,
- Opinion n° 13 of the European Group on Ethics,
- Declarations, Considerations and Guidelines from the World Medical Association on Patient's Rights, Telemedicine, Health Databases, and Medical research involving Human subjects.

- It was demonstrated that the service provider is a processor (sub-contractor) of the data processing's controller. The controller and the processor must be legally or contractually bound (it implies that only well-identified partners operate the applications). The medical data should be processed by a health professional subject to professional secrecy, *or* by another person subject to an equivalent obligation of secrecy, *or* by individuals or bodies working *on behalf* of a health care professional (like a processor) and also subject to such secrecy obligations. These results are relevant and may be extended to all similar GRID-based applications in the health care sector.

The obligation of having a legal or contractual binding link between the controller and some of the subcontractors of the processor might be difficult to manage except if the GEMSS applications are operated by well-identified partners (e.g. use of a trustmark identifying the sub-contractors). There is also the obligation to process medical data by a health professional subject to professional secrecy or by another person subject to an equivalent obligation of secrecy or by individuals or bodies working on behalf of health care professionals also subject to such secrecy obligations.

Two reservations have to be mentioned: *First*, the European privacy rules allow differences between national privacy policies of the Member States. But these differences cannot prevent the transfer of personal data between Member States if the Member States have transposed the European Privacy Directives into their national laws. *Secondly*, as explicitly mentioned in their title, European privacy rules focus only on the protection of privacy. Consequently, if privacy reasons others than the one's indicated in the European Privacy rules cannot prevent personal data processing or personal data transfers between Member States, other reasons such as Deontological reasons, Public Health reasons, Social Security Reasons, etc. can still be in conflict with these operations. With regard to these potential obstacles, there are no practical legal remedies today.

Two remedies can be suggested with regard to this issue: *First*, identify the potential obstacles in each Member States and try and propose European solutions. *Secondly*, establish codes of conduct explaining the use of GEMSS applications, persons and bodies involved with their functions and duties, and clearly describing the patient's rights. On short term, the second remedy should be encouraged rather than the first one. The first remedy should be considered only in the long term.

3.2.2.2.2 Contractual approach

- Considering the provision of services throughout Europe from a contractual point of view, two questions had been addressed :

- 1° What is the content of the contractual obligations of the contracting parties?
- 2° Is it possible to conclude a contract by electronic means?

3.2.2.2.2.1 *The content of the contractual obligations of the contracting parties*

The content of the contractual obligation of contracting parties depends on the applicable law.

The determination of the applicable law to the contractual obligations of the contracting parties, for the provision of GEMSS services, depends on several rules of conflict of laws.

Sometimes these rules of conflict of laws have different natures:

- 1° There are "classical" mechanisms of Private International Law for the determination of the applicable law to the contractual obligations of the contracting parties. An example would be the traditional rule stated by the Convention of Rome, where the contracting parties have the freedom to choose the applicable law to their contractual obligations with some exceptions. If the parties have not made any choice, the Convention of Rome has created subsidiaries rules of conflict of laws.

2° There are also European Community “quasi-“ uniform material rules, related to legal aspects interested in the contractual aspects of the provision of the GEMSS services when trying to harmonize the laws of the Member States through the adoption of Directives.

Some of these “quasi-“ uniform material rules are even accompanied by classic rules of conflict of laws.

The mix of different rules of conflict of laws from different natures is quite confusing when trying to define the content of the contractual obligations of the contracting parties, for the provision of the GEMSS services.

This constitutes a major obstacle for an easy and low-cost day-to-day provision of the GEMSS services involving partners located in different Member States. Indeed it implies that the partners must invest energy and money to know the content of the applicable laws and therefore to understand the real content of their contractual obligations.

With respect to this, it is also useful to remind that it is widely stated that the diversity of contract laws in Europe is a major obstacle to the European Market.

However, the adoption by the European Union of “quasi-“ uniform material rules is definitely a very good step to support the provision of services such as the GEMSS services, even if small discrepancies between national regulations exist.

The simultaneous use of “quasi-“ uniform material rules with other mechanisms of Private International Law does increase the difficulty in defining the content of the contractual obligations for GEMSS partners, and therefore the cost of these services.

With respect to this, the indication of the applicable law by a classical mechanism of Private International Law is not an efficient solution to determine the content of the contractual obligations, even based on the choice of the contracting parties. Indeed, excepted for special cases, at least one of the contracting parties will have to consult a lawyer specialized in the chosen law to fully understand the content of her contractual obligations. This is quite feasible for important international trade contracts, but not so feasible for the provision of medical imaging services throughout Europe.

All these issues require the intervention of very specialized lawyers.

Hence the writing of a contract for the provision of the GEMSS services is a tricky thing with a lot of legal uncertainty, accentuated by the existence of numerous mandatory rules specific to each Member States concerning the Health Sector. These rules are generally ignored by the foreign contracting party e.g. Medical Law, Funding of the health cares, etc.

3.2.2.2.2 Contracts concluded by electronic means

Due to the adoption of Directive 99/93 on a Community framework for Electronic Signature and of Directive 2000/31 on Electronic Commerce, it is possible to consider that, in the extent of the conditions imposed by these directives, contracts may be concluded by electronic means for the provision of the GEMSS services.

- It results from the legal analysis that it is not easy to define the content of the contractual terms for the provision of the GEMSS services on a day-to-day and low cost basis. On the contrary it may be stated that it is easy to conclude a contract by electronic means for the provision of the GEMSS services.

These conclusions aim to suggest possible remedies to this first issue.

Numerous works have already been conducted to study this problem related to the disharmonies between national contract laws in Europe. Some of them have suggested practical solutions to solve these disharmonies.

With respect to this the Principles of UNIDROIT related to the contracts for international trade have to be reminded. Nevertheless these are not suitable for the provision of the GEMSS services.

On 26 May 1989 the European Parliament has adopted a resolution considering the beginning of the study of a European Code of Private Law (Resolution of the European Parliament of 26 May 1989, C/401 of 26 June 1989).

In 2002, the Pavesan Project has published the first part of a draft of a European Code of Contracts Professor GANDOLFI has started his collective work with a list of queries to the members of his group after a first meeting in Pavie in October 1990 (cf. GANDOLFI, G., dir., *Code européen des contrats, avant-projet, livre premier, I*, Académie des privatistes européens, Giuffrè Ed., Italy, Milan, 2002, 576 pages).

The same Resolution has also stimulated another group of legal studies that has published the *Principles of European Contract Law*, under the direction of Professor Carlo CASTRONUOVO (Italy, Giuffrè Ed., 2001, 597 pages).

In 2003 the European Commission has launched her 2003 Action Plan concerning the European Law of Contracts (*Droit Européen des Contrats plus coherent – Un plan d'action*, COM (2003) 68 final).

In 2003 the European Commission has also published a Green Book on the transformation of the Convention of Rome in a Community instrument and on its modernization.

Some authors state that the harmonization of the contract laws of the Member States is not essential to the construction of the European Market (cf. Fr. TERRE, Ph. SIMLER & Y. LEQUETTE, *Droit civil, Les obligations*, Paris, Dalloz, 7^e éd., p. 47, n° 42). They think that the harmonization of national contract laws in Europe should be limited to international contracts (international characteristic due to the nationality of the contracting parties, to the localisation of a pertinent element of the contract, etc.). This approach claims to be compliant with the principle of “subsidiarity”. They suggest that this harmonization should take the shape of uniform material rules (Fr. TERRE, Ph. SIMLER & Y. LEQUETTE, *o.c.*, p. 48, n° 42 *in fine*).

Considering these opinions and considering the provision of medical imaging services through the Internet using Grid technology and involving partners located in different Member States, two possible remedies should be considered.

- 1° The adoption of a Regulation covering the creation of uniform material rules for all the contractual aspects concerning the provision of such services within Europe.

This would be the perfect solution to permit the use of the GEMSS services on a day-to-day basis at the lowest cost.

- 2° To use a model of contract referring to a corpus of rules easily accessible to the contracting partners (on a similar idea, cf. Droit Européen des Contrats plus cohérent – Un plan d'action, COM(2003) 68 final, p. 26, n° 89 & s.).

However the problem of the existence of mandatory rules specific to each Member States concerning the use of Grid technology for the provision of medical services still remains. In order to evaluate the importance of this last obstacle it could be very useful to ask to each Member States to inform the Commission on its specific mandatory rules preventing the use of medical services using Grid technology via, for example, the National Council of HealthCare Practitioners and the national Ministries of Public Health and Social Security.

The legal work provides a skeleton of contract based on the European rules concerning the contractual terms for the provision of medical imaging through the Internet based on Grid technology. This contract should be fulfilled according to the applicable laws when using the GEMSS services throughout Europe.

3.2.2.2.3 Liability approach

- The legal work considers the liability aspects when using such HealthGRID tools regarding European Law.

It aimed at :

- 1° presenting the European rules interesting the liability aspects of the provision of GEMSS services;
- 2° giving a global view on the liability aspects for the provision of GEMSS services regarding European Law;
- 3° providing a conclusion and suggesting possible remedies.

- Several legal instruments may concern the liability aspects when providing Grid-enabled Medical simulation services:

- 1° The European Convention on products liability in regard to personal injury and death;
- 2° The Council Directive 85/374/EEC of 25 July 1985 on the approximation of the laws, regulations and administrative provisions of the Member States concerning liability for defective products;
- 3° The Directive 2001/95/EC of the European Parliament and of the Council of 3 December 2001 on general products safety.

- The producer is liable for damage caused by a defect in his product regarding Directive 85/374.

1. This assertion focuses on industrially produced movables.
2. The injured person has to prove:
 - the damage;
 - the defect;
 - the causal relationship between the defect and the damage.
3. When several persons are liable for the same damage, the injured person is entitled to full compensation for the damage from any of them.
4. The defect has to be determined by reference to the lack of the safety which the public at large is entitled to expect.
5. The producer is not liable in several cases as, by example, when he did not put the product into circulation or when the objective state of scientific and technical knowledge, including the most advanced level of such knowledge, at the time when the product in question was put into circulation was not such as to enable the existence of the defect to be discovered. The knowledge must have been accessible at the time when the product was put into circulation.
6. Compensation may be asked for:
 - death;
 - personal injury;
 - damage to property – limited to goods for private use or consumption.

Under directive 85/372 there is no compensation for pain and suffering and other no material damages payable where appropriate under the law applicable to the case.

7. There is a limitation period under Directive 85/374 for the recovery of damages from the day on which the plaintiff became aware or should reasonably have become aware of the damage, the defect and the identity of the producer.

The right of the plaintiff to compensation is extinguished ten years from the date on which the product was put into circulation.

- In conclusion there is harmonization in European Law concerning the liability aspects for the provision of the GEMSS services regarding defective product – even if this harmonization does not include compensation for pain and suffering and other no material damages.

This harmonization does no more cover the liability relative to the provision of the services provided notably to the patient.

In order to fully appreciate the liability issue regarding the provision of the GEMSS services, the partners should considered all the legal possibilities to be attacked in case of damage. It requires to study first the international jurisdiction of the States where the suit could be introduced (forum convenience) and then to analyze the law applicable to the suit. This kind of legal consultancy is very expansive and takes a lot of time.

On this other hand if the funding of this kind of legal consultancy may be considered for simple situation inducing huge financial return, it seems to be inappropriate for the provision of the GEMSS services on a day-to-day and low cost basis.

Numerous works have already been conducted to study the problem related to the disharmonies between national Tort Laws in Europe, notably by the European Centre of Tort and Insurance Law (www.ectil.org).

ECTIL edits the serie of PRINCIPLES OF EUROPEAN TORT LAW comprising today the following studies:

- Vol. 1: J. Spier (ed.), *The Limits of Liability: Keeping the Floodgates Shut* (1996);
- Vol. 2: J. Spier (ed.), *The Limits of Expanding Liability: Eight Fundamental Cases in a Comparative Perspective* (1998);
- Vol. 3: H. Koziol (ed.), *Unification of Tort Law: Wrongfulness* (1998);
- Vol. 4: J. Spier (ed.), *Unification of Tort Law: Causation* (2000);
- Vol. 5: U. Magnus (ed.), *Unification of Tort Law: Damages* (2001);
- Vol. 6: B.A. Koch/H. Koziol (eds.), *Unification of Tort Law: Strict Liability* (2002);
- Vol. 7: J. Spier (ed.), *Unification of Tort Law: Liability for Damage Caused by Others* (2003);
- Vol. 8: U. Magnus/M. Martin-Casals (eds.), *Unification of Tort Law: Contributory Negligence* (2004);
- Vol. 9: W.V.H. Rogers (ed.), *Unification of Tort Law: Multiple Tortfeasors* (2004).

ECTIL also edits the results of research projects:

- Vol. 1: M. Faure/H. Koziol (eds.), *Cases on Medical Malpractice in a Comparative Perspective* (2001);
- Vol. 2: W.V.H. Rogers (ed.), *Damages for Non-Pecuniary Loss in a Comparative Perspective* (2001);
- Vol. 3: U. Magnus (ed.), *The Impact of Social Security Law on Tort Law* (2003);
- Vol. 4: B.A. Koch/H. Koziol (eds.), *Compensation for Personal Injury in a Comparative Perspective* (2002);
- Vol. 5: M. Faure (ed.), *Deterrence, Insurability and Compensation in Environmental Liability. Future Developments in the European Union* (2003);
- Vol. 6: T. Schobel, *Der Ersatz frustrierter Aufwendungen. Vermögens- und Nichtvermögensschaden im österreichischen und deutschen Recht* (2002);
- Vol. 7: Jos Dute, Michael G. Faure & Helmut Koziol (eds.), *Liability for and Insurability of Biomedical Research with Human Subjects in a Comparative Perspective* (2004);
- Vol. 8: Jos Dute, Michael G. Faure & Helmut Koziol (eds.), *No-Fault Compensation in the Health Care Sector* (2004);

- Vol. 9: W. van Boom, H. Koziol & Ch. A. Witting (eds.), Pure Economic Loss (2004);
 - Vol. 10:H. Koziol/J. Spier (eds.), Liber Amicorum Pierre Widmer (2003);
 - Vol. 11:B.A. Koch (ed.), Terrorism, Tort Law and Insurance (2004);
 - Vol. 12:H. Koziol/W. Doralt (eds.), Abschlussprüfer. Haftung und Versicherung (2004).
- Considering the special characteristics of the provision of GEMSS services only the adoption of a Regulation dedicated to HealthGRID is of nature to solve this important problem.

3.2.2.2.4 Ethical considerations

This analysis aimed at the introduction of ethical considerations relevant to the application of new technologies in Healthcare. The documents highlight the main ethical principles to consider when introducing new technologies such as Grid in Healthcare. Patient rights and their protection are central topics. The following important issues were identified as relevant in the context of electronic health services.

The patient has the right to:

- 1) have an health education to be able to make informed choices. It's important for the patient to have the sufficient knowledge to understand all the information received from the media or other sources. It's a way to reach the auto-determination of the patient who, without adequate information, is unable to point out his needs.
- 2) have access to healthcare. The right covers both transportation and financial capacity. It is important that patients, poor or rich, physically/mentally disabled or not, have equal access health services. By the introduction of the Internet in healthcare, we have to be aware of the problem of its accessibility. In fact, the Internet connection is not available everywhere. The gap between rich and poor population is growing due to the cost of such connection. The problem is the same about the physically/mentally disabled who can encounter huge problems in the access to information accessible through the Internet.
- 3) be informed about his health, the therapy, etc. This right is already reminded in several legislations in Europe but has to be repeated in the ethical approach. The delivered information must be given in an understandable way and understood by the patient, otherwise it's useless. This right is, naturally, connected with the first one.
- 4) give or deny his consent after having received all the required information (cfr. supra). Corollary, he has the right to withdraw his consent at any time without motivation while conserving his right of receiving proper healthcare. The last point is fundamental for the next issue.
- 5) have a pertinent and secure record containing his health data.
- 6) have his dignity respected - such that dignity also covers the respect of the religious believe.
- 7) receive optimal care with respect to the state of the art.

3.3 Workpackage 3: Medical Simulation System

This workpackage had the main task of providing access mechanisms for the GEMSS end users and integrating all the components together into a single system. Before launching into the construction of GEMSS, this workpackage investigated the different means of providing ergonomic end-user access.

3.3.1 Sub-task 3.1: Portals and Access

Sub task 3.1 concentrated on its core objectives of surveying alternative technologies and creating a lightweight framework for incorporating all the client side components. The first objective was pursued by IDAC, ISS and NEC, while the second objective was pursued by ISS and NEC.

For the purposes of the survey work, three technologies were chosen for evaluation:

1. Web Services,
2. OGSA and
3. Unicore.

Then a template containing a standard set of questions was developed and applied to each of these technologies in turn. IDAC undertook the evaluation of Web Services, ISS evaluated OGSA, and NEC evaluated Unicore. During the course of the evaluations, IDAC, ISS and NEC each deployed a simple testbed for the technology they were surveying; hence, this was not a pure theoretical evaluation, but one based on actual (albeit limited) experience. The results of the survey work were described in deliverable **D3.1a** which was completed in mid December 2003.

Work on the light weight, client side framework continued throughout the second year of the project, cumulating in the final release of the framework as described in deliverable **D3.1b**, which was finished in August 2004. During this time period NEC designed and implemented a framework for containing the client side components and providing the applications with a basic interface into the GEMSS environment. The client framework automatically locates and instantiates all client side components, as well as providing communication and security mechanisms for the components and applications. The framework was implemented using an iterative design-develop-evaluate cycle in which features were added over the course of several iterations. This enabled the early release and use of the software by the other software developers.

While NEC was developing the client side framework, ISS developed several key components, namely, the *Basic QoS proxy* and the *Discovery* component. The *Discovery* component, which was finished in March 2004, enables applications to discover new GEMSS services by contacting a known service registry. The *Basic QoS proxy*, which was released in August 2004, allows applications to query the server about basic QoS properties. Both of these components are fully described in deliverable **D3.1b**.

3.3.2 Sub-task 3.2: System Integration and Testbed Deployment

Integration Methodology:

The work and actions of this subtask has been internally organized by an implementation and integration plan. The involved partners (ISS, ITN, and NEC) defined deadlines for both the development of software packages and their integration into the GEMSS environment. This approach allowed the testbed functionality to improve incrementally over the project duration. It also provided the project partners with a clear picture about current and future installations. The alternative approach of having only very few releases, say an initial and a final version, had been dropped, since the consortium identified the following risk: the final version might suffer from unforeseen problems that could lead to significant delays. In particular, the important evaluation activities are dependent on the availability of a running GEMSS environment to perform their actions. Since these tasks require the allocated period of time, the project would have risked running into severe problems. However, in the incremental approach the delay of a (final) version would simply mean that only some functionality is missing and thus limiting the overall risk to a manageable extent.

Testbed Deployment:

Initial Phase: Already for the first review in November 2003, the involved partners achieved to set up and demonstrate an early demonstrator of the GEMSS environment. This environment was installed at the PC cluster systems at ISS and NEC. The initial version contains functionality to upload compressed input data from the client to the server, to start a particular GEMSS application and to download compressed result data after job termination. Already at this early stage SSL security and message level signatures are part of the GEMSS environment. The resource scheduling system is used only for simple job submission and execution operations. A component framework on client side is used to dynamically manage the client entities. At this stage two applications were integrated in the environment.

Phase 2: In February 2004, all GEMSS applications were finally integrated. Additionally, optimizations for large data support were considered and implemented in order to reduce the time for moving data between client and server entities. Another important issue at that time was stability. Since in a real world setting issues like reliability and stability play a key role, we defined a robustness test scenario. The robustness test was designed to test each of the six applications, and the infrastructure, over an overnight period of 19 hours. The cluster at NEC was cleared of its usual jobs for a 19 hours period, allowing GEMSS testers exclusive access. All six applications were then started off, running in non-interactive batch mode, each running with a single test dataset. Each of the applications submitted jobs sequentially, waiting for the first job to finish before submitting the next. Only two jobs failed for reasons that are not directly linked to the GEMSS software. In essence we can state that the GEMSS prototype testbed already demonstrated a considerable degree of stability in this early phase of the project.

Phase 3: Much effort went into the implementation and deployment of this phase. The current testbed is extended by a basic negotiation and QoS module. The QoS module itself is strongly linked to the resource scheduling system in order to query possible – future - allocations (→

advanced reservation). The negotiation module selects the most appropriate offer relative to a underlying protocol. Additionally, security was further improved introducing end-to-end message level encryption, the so called advanced security. The testbed includes services deployed at servers at CCRLE and ISS.

Phase 4:

The phase 4 technology demonstrator has been developed until the end of the project. It now contains the advanced negotiation, process-based access control, accounts service and business module software components. The phase 4 client has been integrated with all the applications, and the server environment installed at both NEC (using the COSY scheduler) and ISS (using the MAUI scheduler). Modifications for the QUARTS application (ST4.2) have been introduced, allowing an interactive batch mode to be setup to support this application's use case requirements. Testing continued until the end of the project.

Known Problems:

System integration has proven to be the most time consuming task for a prototype release since it involves cross-partner co-ordination and the use of developed modules previously untested by the partners. Initial prototype integration involved sequential integration, where one partner would integrate a developed code module and pass the integrated system on to the next partner. This proved inefficient as the project progressed, so for the later prototypes we have moved to using a co-ordinating partner and parallel integration threads. The resulting procedure was highly efficient.

The functionality of each module is summarized in the ST1.2 section, and described in full detail in deliverable D1.2b. A number of lessons have been learnt from the early prototypes. These lessons include:

1. Identifying a single partner to co-ordination integration of the client and server work.
2. Revision of the server build environment to support easier integration of new modules.
3. Revision of client and server build scripts to automate unpacking and use of new module distributions. Automation will remove human error when copying jar files etc to their appropriate locations.

Application Integration:

The task of application integration has been taken on by ISS and NEC and each of the application developers. Each application developer generated, per service provider, a set of scripts to start a job, get the status of a job and kill a job. In addition application developers generated a performance model that ISS's QoS software can invoke to estimate execution time for specific jobs. Application integration has proved less time consuming than the infrastructure module integration, with the application developers evolving their scripts and performance models once the initial work of understanding what is required has been completed.

3.3.3 Sub-task 3.3: Grid-based Support and Consulting

Work carried out:

The goal of subtask 3.3 was to evaluate COTS collaborative tools and teleconferencing software. Sixteen tools were evaluated in total. A number of subjective and objective criteria were chosen with which to evaluate the various support and consulting tools as follows:

- Installation,
- Ease of use,
- Cost,
- Availability,
- Compatibility,
- Security,
- GRID Features.

The tools were subdivided into the following subcategories:

- Remote Control Applications,
- Web Conferencing,
- File Sharing & Groupware and
- Complementary Tools.

All tools were evaluated by IDAC staff and a record was kept of the results and included in the report. A number of recommendations were made after the evaluation had finished. These were based on IDAC's viewpoint as an SME and may not be appropriate to other organizations. A table was also drawn up showing the cost of each tool. The results have been summarized in a restricted report, deliverable D3.3, at project month 24.

The tools most used both with project partners and external users are:

- GoToMyPC – Remote access for PC's in various locations.
- GoToMeeting – Meetings with other members of the consortium (e.g. University of Sheffield)
- WebEx – Used for meetings with clients.
- EASA – Used for testing the GEMSS infrastructure and deploying and demonstrating vertical applications to clients and potential clients.

One area where IDAC did not succeed to find a satisfactory product during the course of the subtask was Voice Over IP (VOIP). Products tested suffered from latency, poor sound quality and often required elaborate firewall configuration to work at all.

Since the end of the task, IDAC have discovered and started using Skype (www.skype.com) for communications between offices. We find this an excellent protocol, call clarity is very good, no noticeable latency and it works over a standard HTTP connection.

3.4 Workpackage 4: Medical Service Applications

This workpackage is responsible for the adaptation and integration of the medical simulation and image processing software into the GEMSS testbed. It includes a variety of medical service applications which

- have different GRID requirements concerning computation time (near real-time requirements vs. standard batch processing), memory usage, encryption, etc. and
- address different medical areas (cranial, pulmonary, cardio-vascular system) to address an end-users group of sufficient size for service provision.

Name	Domain	Class	Users
Maxillo-facial surgery simulation	Medicine - pre-surgical planning	Distributed supercomputing / On demand	Medical doctors, researchers
Neurosurgery support	Medicine - intra-operative planning	On demand	Medical doctors, researchers
Radiotherapy planning	Medicine - Monte Carlo treatment simulation	On demand / distributed supercomputing	Medical end-users; Doctors, researchers
Inhaled drug delivery simulation	Medicine - air flow dynamics	On demand / distributed supercomputing	Medical end-users; Doctors, researchers
Cardio-vascular system simulation	Medicine - blood flow dynamics	On demand	Medical end-users; Doctors, researchers
Advanced image reconstruction	Medicine - nuclear / in vivo diagnostics	On demand	Medical end-users; Doctors, researchers

Figure 3.11: Classification of the 6 GEMSS Medical Service Applications

3.4.1 Sub-task 4.1: Maxillo-facial Surgery Simulation

Medical background:

In patients suffering from severe maxillary hypoplasia and retrognathia (see Fig. 3.12 left), conventional therapeutic surgery often fails to guarantee long-term stability. Using a rigid external distraction system (Fig. 3.12 right) for midfacial distraction osteogenesis is a new method to correct the underdevelopment of the midface, surpassing traditional orthognathic surgical approaches for these patients. Currently surgical planning is only based on CT images. The treatment consists of a midfacial osteotomy (bone cutting) followed by a halo-based distraction (pulling) step. The goal of this sub-task is the modeling of the distraction process for individual patients to allow predictions on its outcome.



Figure 3.12: Patient before operation (left) and after operation, with distraction device mounted (right).

(Photographs courtesy of Dr.Dr. Th. Hierl, University clinics Leipzig)

Tool chain outline:

A simulation of the maxillo-facial surgery involves a considerable number of individual tasks, which are generally outside the surgeon's expertise. Therefore, emphasis has been put on automating this chain as far as possible. The steps of the planning simulation are as follows:

- The image data of the patient is acquired (typically CT, in DICOM format).
- The image data is converted into a format understood by the tools (Vista format) and interpolated to isotropic voxels.
- The image is segmented into bone and (one or several kinds of) soft tissue. Alternatives are using a thresholding approach and using a template-based registration approach.
- A surface mesh of the bone is generated.
- The surgeon interactively specifies bone cuts and displacements on the surface mesh (virtual osteotomy).
- The cuts and displacements are used to create a 3D finite element (FEM) model of the problem that is based on the medical image of the patient. This includes mesh generation and application of boundary conditions.

- The FEM problem is solved by a simulation code.
- The results are visualized and interpreted by the surgeon.



Figure 3.13: Volume visualization of CT image of patient' head, before surgery (left) and simulated result after surgery (right).

(CT data kindly provided by Dr.Dr. Th. Hierl, University clinics Leipzig)

Workflow:

As the toolchain consists of several independent tools, some means of coupling them has to be applied, as well as some means of allowing the user to interact and customize the workflow. We chose the Triana workflow editor [1] for this purpose. The individual tools have been wrapped into Triana units, forming building blocks for constructing

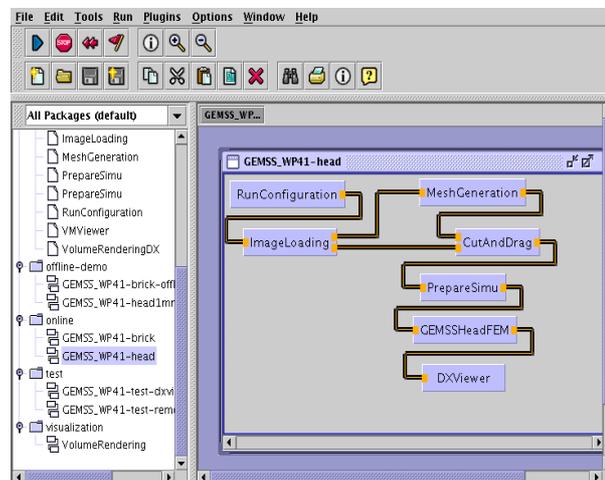


Figure 3.14: The Triana workflow editor represents the top level user interface

toolchains using a graphical programming language. Our toolchain contains three major points of user interaction: First, the (optional) rigid and non-rigid registration, but also enhanced segmentation requires the definition of landmarks on the rendering of skull and skin surface. Second, and most important, the surgeon has to define the surgery operation by specifying cuts and displacements. And finally, the results are visualized. Between these interaction points, substantial data processing is going on. Therefore, we have defined several chains which allow the job to resume execution at a later stage, without having to wait for the next interaction.

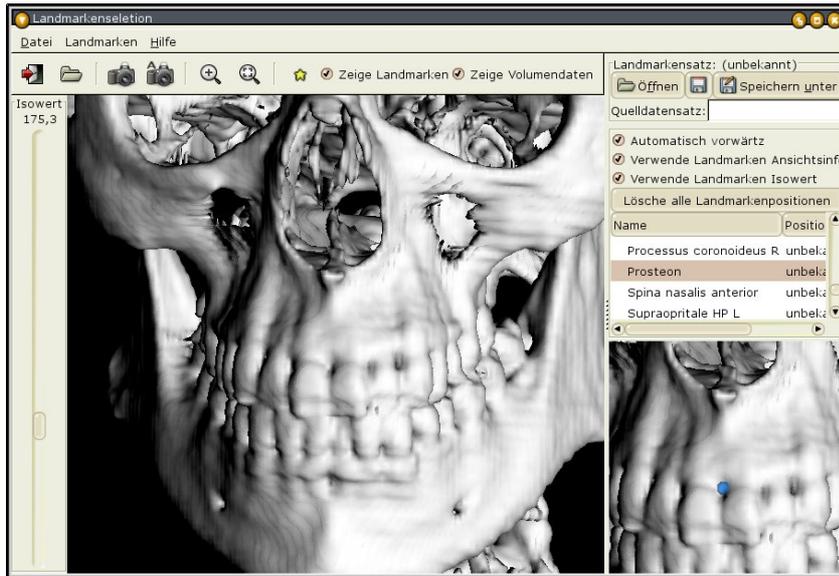


Figure 3.15: The landmark picking tool. The user is guided by images from a model geometry.

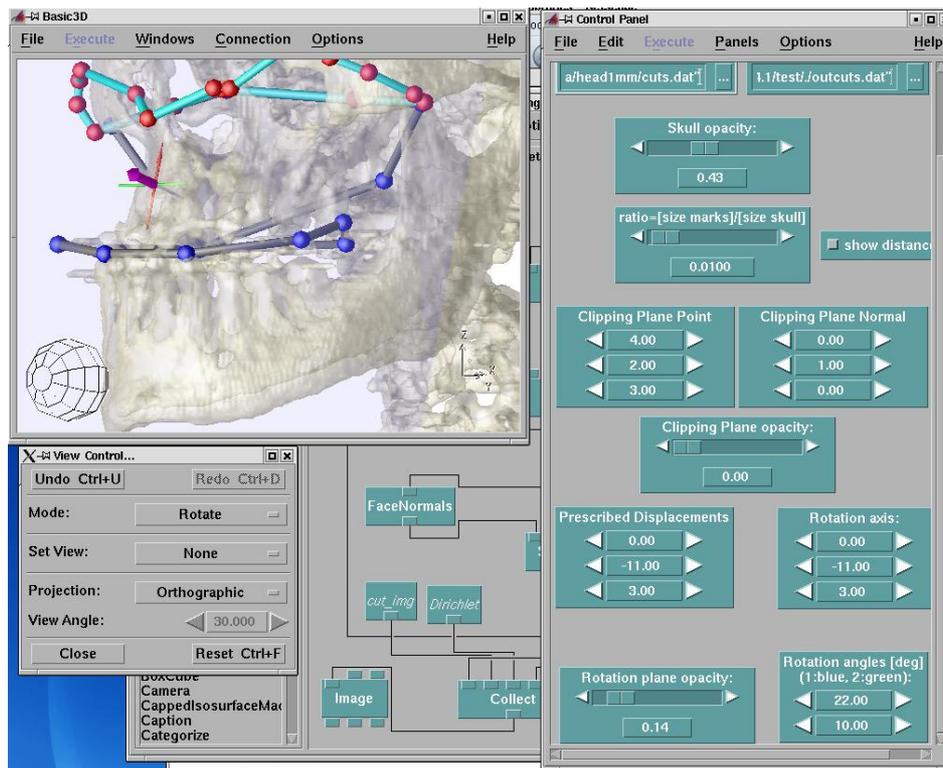


Figure 3.16: The virtual osteotomy (bone cutting) tool. A surgeon may specify several cuts. The lower cut separating the teeth may be necessary to overcome segmentation artifacts; new tools help avoiding such artificial cuts.

Grid enabling:

The task with the largest requirements of computer resources is clearly the FEM simulation; it has to be carried out on a remote high-performance computing (HPC) platform, unless one can accept a rather coarse approximation. Other tasks like mesh generation and non-linear registration are also demanding, but for the currently used image and mesh sizes these tasks still can be carried out on the client side. In principle however, they are also eligible for

remote execution. This scenario can be termed *thick client*. A different scenario is called *thin client*, where everything runs on the server, and the client uses a remote control tool like VNC to connect. A variant of this solution, running the VNC server on the client, has been implemented to provide remote assistance to our medical partner at University Clinics Leipzig.

In order to provide Quality of Service (QoS), data has been gathered allowing the prediction of the runtime and memory consumption of the remote FEM solver. A performance model has been developed, implemented and integrated into the GEMSS QoS framework. During execution of the remote simulation, the client can query continuously its current status and get an updated estimate of the remaining time until completion.

Evaluation and Test cases:

Synthetic tests have been set up allowing quick tests of client and server functionality. These tests consist of a scalable brick (of "bone") surrounded by soft tissue. They are also used to study the numerical behaviour of the solver.

In order to ensure clinical testing and evaluation by a medical practitioner, a collaboration agreement has been signed with Dr. Hierl, Department of Oral and Maxillofacial Surgery, University Clinics Leipzig. A Linux workstation equipped with the client software has been installed at Dr. Hierl's office. Several improvements suggested by Dr. Hierl have been incorporated into the toolchain.

A graphical landmark-picking tool has been implemented allowing the definition of currently 33 different landmarks on the patient's skull and skin. The set of landmarks is easily extensible and can be adapted to future needs. By using landmarks, a rigid registration of the non-moved parts of a patient's head on pre- and postoperative CT scan is performed, as well as a determination of the actual displacement of the maxilla. Using landmarks on moved soft tissue permits quantitative measurements of the simulation errors.

As mentioned before, creating an *automated* toolchain is of utmost importance for the successful adoption of such a simulation-based surgery planning application by the medical community. Creating such an automatic chain faces a number of challenges. With standard segmentation techniques, it is not possible to guarantee a topologically correct segmentation, for instance, to ensure separation of upper and lower teeth. The cuts specified by the surgeon must be guaranteed to indeed separate the maxilla from the rest of the skull. Also, metal artifacts distort the model. We have developed tools to deal with these obstacles, including a non-linear registration approach. However, non-linear registration is rather time consuming and may have difficulties if the differences between the segmentation template and the patient are large. A set of alternative tools has produced promising results, but still needs to be tested on a larger number of medical cases.

The next prerequisite for a stable simulation (especially in the non-linear case) is the generation of a suitable mesh. We found several conditions that a mesh must fulfill for stable non-linear simulation, starting from the most obvious restriction to a single connected component, and developed corresponding mesh filters. Linear simulations are much more robust in this respect.

Effort has also been put into making the numerical solver more robust, e.g. by automatic timestep adaptation to avoid convergence failure. In general, making a (nonlinear) solver robust requires a number of advanced techniques like remeshing and automatic parameter and algorithm selection, which are beyond the scope of this project. We believe however, that these issues are critical for the success of application scenarios like ours, where simulations are run by non-experts.

End-user evaluation:

End-user evaluation was done by our cooperation partner at the University Clinic of Leipzig. Surgeon Dr. Dr. Th. Hierl was provided with a desk-top computer running the GEMSS client software for usage in his maxillo-facial surgery planning. Several improvements were implemented according to his advice and Dr. Hierl expressed his satisfaction with the resulting planning tool.

Details of developments:

A complete version of the toolchain is running at several sites, including a clinical one. The requirements listed in D1.1 are fulfilled. The following section gives a detailed overview of all the components developed within subtask 4.1.

Compliance to standards:

- Tools to import DICOM [3] images have been implemented
- Compliance to the X.509 standard via the GEMSS security infrastructure

Grid integration:

- Full integration as a Grid service into the GEMSS system
- Development and integration of a performance model predicting runtime and memory consumption of the remote FEM solver (for the linear elastic model)
- Server-side extraction of job status information and completion time estimation which is transferred to the client
- Server-side tests to detect error conditions such as cluster hardware failures

The following tools have been implemented:

Image processing:

- Segmentation of 8bit and 16bit images into 3 or 4 classes (bone, soft tissue and optionally muscles)
- Tool to remove or reduce metal artifacts
- Rigid registration based on landmarks for quantitative evaluation
- Landmark-based non-linear registration implemented as alternative to threshold based segmentation
- Tool for applying cuts to an image, thereby ensuring the separation of components of interest, specified by landmarks

User interaction:

- Using the Triana workflow editor, a top-level GUI for the entire toolchain was created, offering several customized workflows to the user.
- An interactive landmark-definition tool with graphical user-guidance
- Interactive cutting tool, supporting the independent displacement of several components, the highlighting of cut volumes and the coloring of connected components

Mesh & model generation:

- Volume mesh generation allowing smooth interfaces between several materials
- Tools to apply various boundary conditions to a volume mesh

Numerical solver:

- Support for hyperelastic and viscoelastic material models
- Adaptive time step control for non-linear solver to increase robustness
- Performance model for predicting runtime and memory consumption of the remote FEM solver (linear elastic model)

Result Visualization:

- Customized visualization environment, based on OpenDX [2]
- Enhanced visualization based on volume rendering (see Fig. 3.13 right)

Conclusions:

The maxillo-facial surgery application has reached a fully functional stage. Feedback from our clinical partner Dr. Hierl has resulted into substantial improvements of the toolchain.

The application is fully integrated into the GEMSS system. Thus, it offers full security and transparent access to remote HPC resources, as well as accounting, billing and QoS guarantees.

It has turned out that fully robust simulation chains are a challenging aim, especially if non-linear processes are involved. We have developed tools to achieve topologically correct segmentation, guarantee valid cutting regions and obtain geometric models suitable for non-linear simulation. These tools greatly enhance the ergonomics of the toolchain. It cannot be yet guaranteed that all potential problems are solved automatically; thus, additional work will be necessary, before the application can enter clinical routine.

We firmly believe that robust simulation chains are possible and that GEMSS has been a decisive step towards this aim. We also are convinced that the superior physical accuracy and modeling capabilities of non-linear methods will justify the additional work required to achieve robust applications. Work on this application will therefore continue; NEC has committed to keep this GEMSS service available beyond the end of the project.

Dissemination:

The GEMSS approach and the toolchain for maxillo-facial surgery simulation have been presented at a number of workshops and conferences, for a complete list of publications and presentations see section 3.8 at the end of this report.

References:

- [1] The Triana workflow editor <http://www.trianacode.org>
- [2] OpenDX homepage <http://www.opendx.org>
- [3] DICOM - Digital Imaging and Comm. in Med., <http://medical.nema.org/dicom/2004.html>

3.4.2 Sub-task 4.2: Neuro-surgery Support

Background:

The major shortcoming of image-guided surgical planning based on pre-surgically acquired functional MRI (fMRI) data is the brain shift phenomenon (See Fig. 3.17). The occurrence of surgically induced deformations invalidates positional information about functionally relevant areas. This problem is addressed by non-linear registration of pre-operative fMR images to intra-operative MRI acquired by an Open-MR scanner, or to intra-operative 3D ultrasound data.

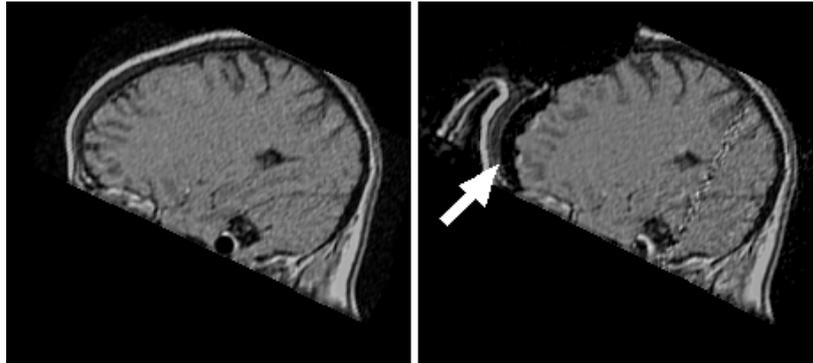


Figure 3.17: Brain before (left) and after (right) opening the skull. Note the brain shift indicated by the arrow.

Workflow and Grid Enabling:

As requirements for the chain to work, a pre-operative MR scan together with its aligned fMR data of the patient is needed. During the first stage of the surgery, before the skull is opened, an usually low-resolution image with the Open-MR scanner is acquired. After the correction of possible RF-Field inhomogeneities a linear registration of this image with the anatomical high-resolution pre-operative data takes place. The registration parameters are stored as starting position for further linear registration steps. The registered image will be the reference for further steps of the chain.

After the opening of the skull further intra-operative images are acquired. These images are also corrected with respect to possible intensity inhomogeneities and registered with the first intra-operative data using the stored parameter set. To gain the same intensity distribution in both input images, a linear intensity adjustment might be made. Then the non-linear registration will be executed. The resulting displacement field of the non-linear registration process is applied to the pre-operative fMR data. In the last step the deformed fMR data will be overlaid to the linear registered open-skull data set and later sent to a presentation device.

The fluid based non-linear registration method produces best results if its input images are originating from the same scanner. That is the reason why the first (closed skull) intra-operative image has been acquired and used as a reference image for further processing and not the pre-operative high-resolution data which is usually not acquired with an Open-MR scanner.

At the beginning of the project, processing time for this chain was about 4 h (Intel Pentium III, single processor). To avoid a too long delay of the progress of surgical intervention, a maximum processing time of approx. 10 min is acceptable. The time-consuming registration steps are readily parallelisable on shared or distributed memory high performance computing platforms that are available from remote service providers. Grid technology allows switching between local and distributed environments easily.

Elements of the Image Processing Chain:

The image processing chain focuses on the registration of low-resolution Open-MR data to low- and high-resolution MR data:

- Data transfer and conversion: Not implemented due to the lack of an Open-MR scanner. Data is expected to be in the machine-independent Vista format. Converters are available which can easily convert images from DICOM in Vista format.
- Correction of intensity inhomogeneities: This step is very time consuming due to the solution of a huge linear system. To improve speed the linear system is only coarsely solved within a multi-resolution framework, which is sufficient to estimate a proper bias field. A further speed improvement was obtained during operating on an enlarged head mask that can be extracted from the given dataset. The biggest improvement of performance was gained by computing the solution of the linear system in parallel. Finally, the algorithm has been enhanced to work in a multiprocessor shared memory environment yielding nearly linear speedup. This was realized by an overlap of iterations: The next iteration is starting as soon as all necessary data has been computed, although the current iteration did not finish yet. This is the reason why the maximum number of usable processors is bounded by the number of slices in the MR image. A different strategy had to be applied in a distributed memory environment. Here, the data set is partitioned into blocks and each block is solved independently from the others.
- Linear registration: The registration of the low resolution intra-operative dataset to a high resolution pre-operative image is realized by maximizing their normalized mutual information (NMI) resp. cross correlation (CC). NMI is used when data from different scanners is going to be registered and CC is used for datasets originating from the same scanner. The registration is done in a multiresolution framework which produces a significant speedup. To achieve a fast convergence, the down-hill simplex optimization algorithm is used, which performs well and does not require any gradient information. To improve speed of the registration, a parallel evaluated speculative down-hill simplex was developed that needs the same number of iterations to converge as the original method, but twice as fast. To reduce the risk of finding local optima instead of the global optimum a parallel evaluated genetic algorithm is used on the lowest multiresolution level. By partitioning the data into blocks and evaluating the cost function (NMI and CC) in parallel, a further, nearly linear speedup was gained. The results of the processed sub volumes are cumulated to obtain the cost function value. All the parts of the linear registration that have been mentioned above can be computed in a shared and distributed memory environment.
- Intensity adjustment of two scans: The result of the non-linear registration step of the processing chain depends, among other things, on the similarity of the intensities of both images. Since this step is not very time consuming, it can be performed sequentially.
- Non-linear registration: To obtain a deformation field that can be applied to an fMRI image a non-linear registration is required. In this chain a method based on fluid mechanics is applied. The time consuming part here is again the solution of a huge linear system of equations. To accelerate its solution and to avoid problems due to local minima a multi-resolution approach is applied. A further speedup is achieved by solving the system in parallel where each processor operates on a single "slice" of the system. For full details see the GEMSS Deliverable D4.2.
- Application of a deformation field to fMRI data: The deformation field obtained by non-linear registration will be assigned to a fMRI dataset by shifting each voxel of the dataset by its corresponding vector from the displacement field.
- Overlay of deformed fMRI data with intra-operative dataset: In this step the deformed pre-operative functional dataset that was initially aligned with the pre-operative anatomical MR scan will be overlaid to the registered intra-operative image to show regions of

activation with respect to the brain shift.

- Conversion and transfer to a presentation device: A graphical user interface (Fig. 3.18) has been developed which shows the results of the image processing chain on a monitor

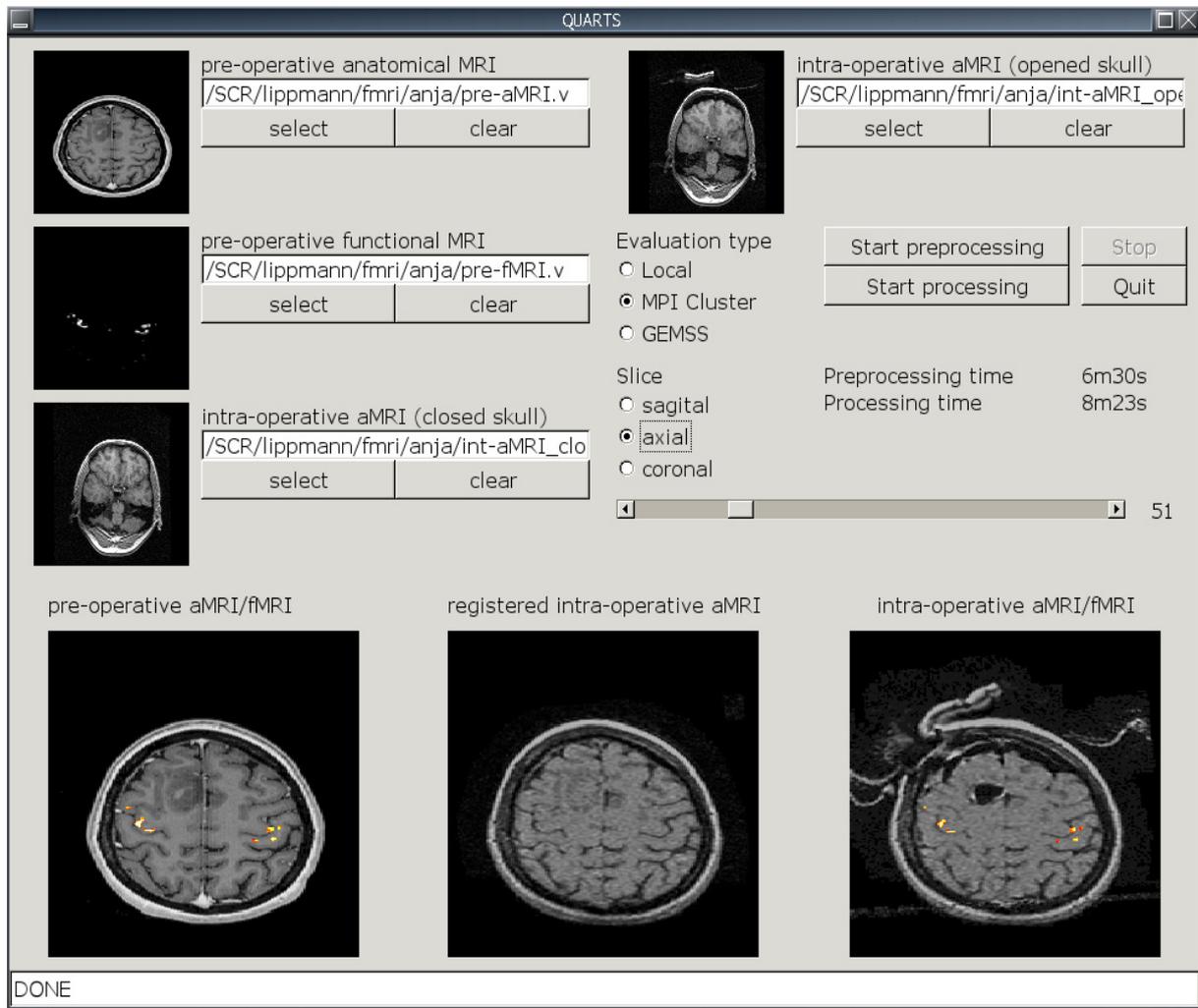


Figure 3.18: QUARTS Client: Images can be viewed and the type of data processing can be selected.

Status Summary:

Due to the requirement of processing the whole chain (including image acquisition) in less than 10 minutes, large computation power is needed. This can be provided through a local cluster with multiple processors. However, these clusters are quite expensive, need maintenance and are often used below their capacity. Instead of a local solution the Grid could be used to execute the compute intense part of the chain as a remote service. For Grid interaction, a local PC or workstation is sufficient.

The image processing chain takes about 10 minutes on a AMD AthlonMP 1.6 GHz distributed memory PC cluster to be executed over the grid using the GEMSS middleware phase 2. To achieve this execution time of 10 minutes 10 to 12 processors have to be applied.

With phase 4 on an AMD AthlonMP 2.1 GHz PC cluster the chain needs less than 10 minutes if 8 processors are used. The run time has been measured using 2 real patient data sets. However, the open MR scanner at the department of Neuro-Surgery of the University of Leipzig - which was available at the beginning of the project – has been removed, and we are, therefore, not able to further conduct an application of the software under real world conditions.

Conclusions:

A Grid-enabled Neuro-surgery Support application is now operating successfully on the GEMSS Grid. Tests have shown that this time-critical problem can be efficiently solved on the GEMSS Grid. The evaluation of the neuro-surgery tool has demonstrated the viability and the advantage of the Grid approach (see mid-term evaluation report, D1.3a, and final evaluation report, D1.3b, for further details).

Dissemination:

The GEMSS approach and the toolchain for quasi-realtime neuro-surgery support have been presented at a number of workshops and conferences. A complete list of publications and presentations is given in section 3.8 at the end of this report.

3.4.3 Sub-task 4.3: Cranial Radio-surgery Simulation

Application Scenario:

Gamma Knife[®] Radiosurgery is a non-invasive medical procedure using beams of ionising photons from 201 ⁶⁰Co sources to treat intra-cranial lesions. The Gamma Knife[®] unit comes with a treatment planning system, GammaPlan[®] that uses an approximate description of the photon interactions within the head of the patient to calculate the energy dose deposited by these photons in the region of the tumour. There is significant benefit to be obtained from improving the fidelity of these calculations, particularly in cases where photons traverse regions of widely differing electron densities (e.g. soft tissue and bone). Monte Carlo modeling can accommodate these complexities and can play a useful role in complementing the GammaPlan solution (with the potential to eventually supersede it in the event of short enough calculation times). The goal of this sub-task is to adapt and Grid-enable a Monte Carlo code (RAPT/EGS4) written for conventional radiotherapy to that of stereotactic radiosurgery. The presence of the Grid enables calculation of the energy dose delivered to the brain from a Gamma Knife[®] treatment unit to be obtained in clinically useful timescales (less than one hour).

Workflow:

The Grid-enabled radiosurgery application uses RAPT as a front end to the EGS Monte Carlo engine to model ionising radiation transport through the head of the patient. It requires:

- Definition of patient geometry
- Specification and distribution of material types contained within the geometry
- Position of beam isocentre
- Beam properties – intensity profile, spectrum
- Beam distribution – number of beams and their arrangement, number of shots etc.
- Quality of simulation parameters – total number of photons, interaction types

This data is specified by the contents of numerous text files that are loaded into the EGS solver at startup. The files are not native to EGS but are created for EGS through use of a bespoke RAPT GUI developed within MatLab. All input files are stored in a default *Input* working directory, zipped, encrypted and dispatched to the Grid. The simulation process simulates the dose given to the region of interest by modelling millions of photons, and following their paths, employing information from photon scattering data, to correctly give the photons their positions, angles of deflection, and energies or to absorb them in the tissue as they interact with the atoms of the target. The energy distribution within the geometry equates to the dose distribution of the model. Thus the output from the modelling process is:

- 3D patient mesh geometry
- Accumulated dose at each element of the solution mesh
- Flux variance at each element of the solution mesh

The results archive is pulled from the Grid in encrypted form and unzipped on the client PC within the working *Outputs* directory. This data is accessible to the user as a set of text files, but a visualisation application has been written within MatLab to enable the user to explore the distribution of radiation dose within the treatment volume. The dose data can be represented as contours on specified planes through the volume mesh or visualised as isosurfaces in 3D. Additionally, the ‘MetriX’ utility has been developed to permit quantitative comparison of plans. This is useful when comparing the merits of different proposed treatments or comparing the dose distribution obtained by GammaPlan or experimental methods with the solution obtained by RAPT.

Grid Enabling:

The RAPT software has been run and tested under LINUX and Windows NT environments. Integration of RAPT with the planning process in radiosurgery has been accomplished by creation of a bespoke GUI targeted for compatibility with GammaPlan. This readily accepts all parameters generated/required by GammaPlan and is able to replicate the treatment scenario. Secure data transfer compliant with the X.509 standard required a Registration Authority appointed in the Medical Physics Department at Sheffield University. A data controller within the hospital has been identified and operation of secure RAPT from within the clinical radiosurgery department has been demonstrated. An important goal of the project is to evaluate the software within the clinical domain, and preliminary clinical example results computed by RAPT are very encouraging (Figures 3.19a and b). The hospital firewall is very tightly monitored, so it is not possible to ‘push’ data from an external source into the NHS network. However, the ability to ‘pull’ the data from within the bounds of the hospital firewall can enable the running of remote Grid jobs from the hospital environment. It is the reliance of GEMSS middleware on Web Services that makes this transaction possible.

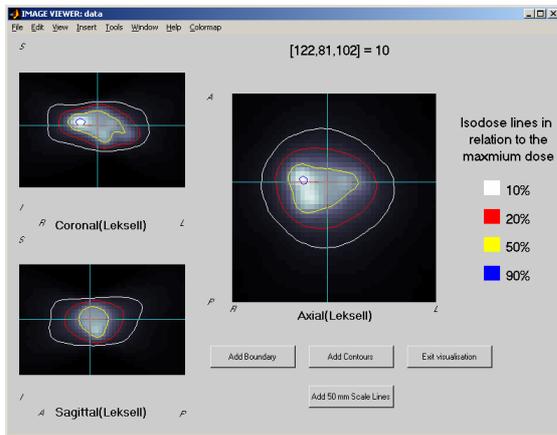


Figure 3.19a RAPT solution for 201 beams of photons
- clinical plan -



Figure 3.19b GammaPlan solution for 201 beams of photons
- clinical plan -

Data security is paramount and utilises 128-bit encryption. The QoS model is designed to let the user specify the time of job completion and uses an estimate of job run time based on benchmark data supplied by preliminary evaluation tests. As expected this is critically dependent upon the number of photons to be processed within the simulation and the number of available processors. Timely solution is critical in this clinical application, and the ability to assess job status by polling the Grid to determine the state of the simulation while it is running helps in this respect. A simple business model is supported by the Phase 4 middleware, and involves negotiation of service provider and cost prior to commencement of each job.

Evaluation: Sample Problems and Test Cases

The utility of the software has been explored through the use of many test cases. These are designed to:

- Confirm accuracy of the RAPT/Monte Carlo solver

- Permit assessment of the efficacy of the RAPT radiosurgery planning process in GEMSS
- Act as a metric by which the RAPT performance can be judged, consolidating QoS benchmark data.

Over 600 jobs have been submitted to the Grid in pursuit of evaluation. They can be broadly grouped into four different categories as outlined below:

- Simulation of radiation transport through water. The quality of the solution can be assessed by determination of the linear attenuation coefficient etc. and comparison with published data.
- Simulation of dose distribution in a spherical head phantom. Evaluation of the quality of solution is through comparison with the GammaPlan computed dose distribution.
- Experimental validation of the computed dose distribution obtained using a spherical head phantom. Evaluation is by comparison of the RAPT solution with the experimentally determined dose data.
- Simulation of dose distributions in clinical treatment plans. Evaluation is through comparison of results between GammaPlan and RAPT.

Many months of evaluation have confirmed that Grid-enabled RAPT is robust and able to produce clinically relevant results of acceptable accuracy (within 2-3%) in under an hour (at least 30 processors are needed - compute time is a function of photon statistics and available processors). Grid reliability averaged in excess of 90% for the month of January 2005 with failure usually due to server maintenance. Investigation of RAPT scalability shows almost linear performance gains for up to 30 processors (Figure 3.20). It is during the evaluation period that several bugs were identified, including one that had its origins in the GammaKnife utilities software supplied by the manufacturer (data corruption in the Leksell extractor tool). All known bugs have since been fixed. Further details are included in the final evaluation report, D1.3b. It is clear (even with Grid assistance) that iterative planning with GammaPlan can not be replaced by RAPT since the latter is insufficiently responsive to provide rapid dose distributions for the iterative planning process (a speed increase of several orders of magnitude is required if RAPT is to compete with the 'real time' response of GammaPlan). However, with solve times of less than one hour clinical experience demonstrates that Grid-enabled RAPT has a valuable role to play in confirming the dose distribution determined by

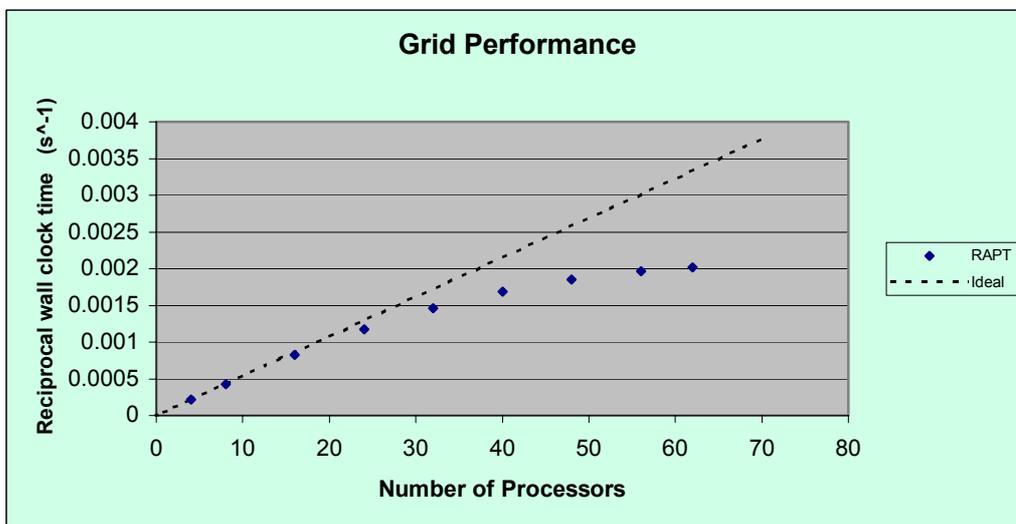


Figure 3.20. Scalability of run times using a RAPT benchmark. The dotted line of the graph illustrates ideal scalability.

GammaPlan, particularly in those circumstances that contravene the radiation transport assumptions inherent within GammaPlan. This means that for the large majority of cases, comparison of dose data computed by GammaPlan and RAPT show consistently good agreement (essential if RAPT is to gain any credibility in the clinical domain), but in the presence of bone/air close to the isocentre, striking differences result. Under these conditions RAPT has the opportunity to have a significant impact upon patient management.

Status Summary:

This summary outlines key features of the GEMSS RAPT service accomplished within the GEMSS project:

- Grid enabled RAPT accommodates all aspects of a clinical treatment plan through an intuitive user friendly interface
 - 201 beams with support for beam plugging
 - Multi-shot treatments
 - Support for Bubble head geometry
 - Arbitrary positioning of isocentre
 - Support for 4 material types (vacuum, air, tissue, bone)
 - Support for calculation of treatment shot times

 - Current principle limitations of RAPT are:
 - 1mm maximum spatial resolution
 - 200x200x200mm target/patient geometry volume
 - No CT/MRI skull geometry support (currently under investigation)

- Documentation is provided with this software, and includes a tutorial guide and supplemental technical information
- A results visualisation GUI has been developed that permits exploration of dose within the head geometry.
- The MetriX utility developed within GEMSS enables direct comparison between RAPT, GammaPlan and experimental dose data from experimental film measurement.
- The RAPT solver has been proven to be accurate and robust
- Solutions utilising in excess of 500 million photons are required for clinical acceptability (statistical errors < 3%).
- Multiple shot treatments with closely co-located isocentres can be solved within RAPT to clinically acceptable accuracy in under an hour (30 processors)
- Comparison of RAPT with GammaPlan and experimental data indicate that RAPT offers improved description of dose in those circumstances in which the assumptions relevant to GammaPlan are contravened.
- Application development has been driven strongly by clinical recommendations. These have influenced the development path of the software (e.g. subsequent creation of MetriX utility).
- The Grid enabled application fulfils the requirements specification of D1.1
- A MatLab licence (version 6.5) is required for the RAPT client.
- The service complies with the GEMSS security infrastructure (X.509 compliant)
- RAPT has been deployed with Phase3 and Phase 4 middleware. In particular, the latter offers:
 - Improved job status control
 - Estimation of solution time (QoS feature – performance model)

- Improved job scheduling (QoS feature - scheduling)
 - Choice of compute server (QoS feature - negotiation)
 - Grid interaction through a well defined and transparent business model
- Extensive evaluation of RAPT has been undertaken, involving:
 - Clinical plans
 - Feedback from the clinical environment
 - RAPT computed dose comparison with known dose distributions
 - Documenting of Grid reliability
 - Documenting of Grid-RAPT performance

Outlook beyond the project:

RAPT has been elected to remain functional as a GEMSS application demonstrator on the NEC Grid server (courtesy of NEC) beyond the end of the project. The interest generated by the software has led the NHS radiosurgery department at Sheffield to arrange for its continued use within the department beyond the end of GEMSS. Consequently, it has been installed on the Medical Physics cluster at the Royal Hallamshire Hospital.

Summary and Conclusions:

Grid-enabled RAPT is operating successfully on the GEMSS Grid. It is apparent that the large Monte Carlo problems encountered in Gamma Knife radiosurgery can be solved effectively through the computing resources provided by GEMSS. The accuracy of the simulation results is a strong function of computation time and resources, and the Grid offers a significant advantage in this respect. Extensive evaluation exercises have demonstrated the utility of Grid enabled RAPT in a clinical environment, and implications for patient management are emerging in cases involving significant tissue inhomogeneity. The tentative acceptance of the RAPT Grid-enabled radiosurgery application within the hospital environment at Sheffield is early vindication of many of the concepts embedded within the GEMSS infrastructure.

Dissemination:

Our dissemination programme includes publications, conference presentations, and demonstrations and representation at the GammaKnife user's conferences (see section 3.8). RAPT can have clinical impact in the radiosurgery environment and therefore continued funding beyond the end of the GEMSS project is being pursued.

3.4.4 Sub-task 4.4: Inhaled Drug Delivery Simulation

Application Scenario

The inhaled drug delivery simulation has adopted the acronym ‘COPHIT’ – ‘Computer Optimised Pulmonary delivery in Humans of Inhaled Therapies’. It is an acronym that emphasises that optimised delivery of medication to the lungs can be achieved by modelling the drug delivery process. Knowledge of the characteristics of the delivery device (eg. inhaler) and the airways is required, as are the airflow and physical characteristics of the medication. These elements determine how medicament is entrained in the airflow and how the drug is deposited on the airway walls. The software allows drug designers or manufacturers of inhalation devices to experiment *in silico* with device geometry, delivery timing, pharmacokinetics or physical formulation of the medication, and thereby maximise anticipated dose to the desired region of the respiratory tract.

Necessarily, this approach utilises a suite of tools, but it is the CFX computational fluid dynamics solver that is the primary means by which such problems are solved. It permits computation of the inhaled flows and drug deposition based on real breathing profile data and real lung geometries obtained from CT scans. However, the solution of inherently complex physiological problems allied to respiration is fraught with difficulties. The presence of Cophit-motivated coupled compartments designed to improve the fidelity of the simulation only complicates matters further. As a whole, such respiratory simulation requires a level of expertise and computing power that makes it completely inaccessible to all but the most expert of users.

It is for this reason that GEMSS offers an Inhaled Drug Delivery Simulation *service*. The ethos of such a service is that the expertise required for this application resides with the developer (e.g. University of Sheffield Medical Physics, or consultancies such as IDAC and ASD). The developer, with the availability of additional tools, is in a position to create a bespoke application tailored to the needs of the customer. This is made possible through the creation of an interface (using EASA) that is able to hide the complexity of the simulation behind a simple point-and-click GUI (Fig. 3.21), but it does require that the problem can be expressed in parametric form.

Workflow

The parametric approach makes respiratory simulation readily accessible to the end user, whilst the Grid meets the requirement for accessible large scale computing resources. It is a powerful combination. The primary disadvantage is loss of flexibility, since users are unable to explore issues that are outside the scope of the GUI that was originally designed for them. Solution of wider problems is possible, but requires construction of a new EASA enabled application. From our experience with EASA, building an application from scratch is a significant undertaking, but subsequent modifications are relatively easy to implement and the modified application represents a new bespoke application for the client (which justifiably could involve additional separate charges, according to the business model used).

The application requires the user to enter relevant data in a series of steps spread over eight data entry screens as follows:

- Screen 1 - Confirm choice of lung mesh geometry
- Screen 2 - Specify time-step information and material properties
- Screen 3 - Specify coupled alveolar compartment properties
- Screen 4 - Specify time varying inlet flow/pressure and substance quantity
- Screen 5 - Specify initial conditions for the 3D flow field
- Screen 6 - Specify pharmacokinetic model parameters
- Screen 7 - Specify the nature of the results to be displayed
- Screen 8 - Choose solver (local or on the GEMSS Grid)

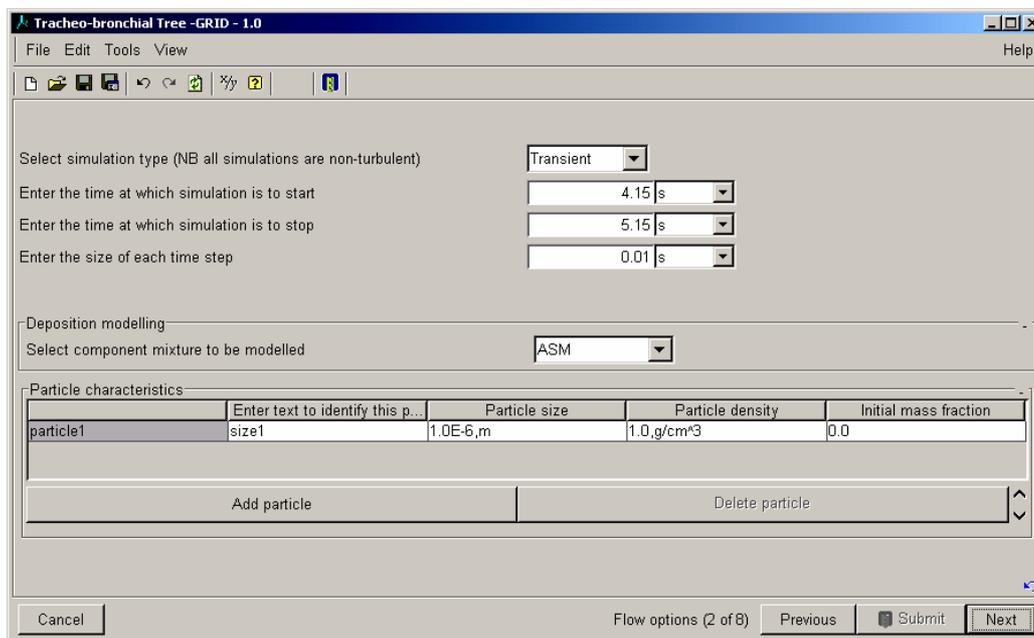


Figure 3.21: An example data entry screen provided by the (EASA-enabled) Cophit GUI

The X.509-based security model of GEMSS protects data transmission between the Client and the Grid server where the computationally intensive fluids problem is solved. The results data is returned to the client and presented in numerical and graphical form. Tools are available for easy visualisation of flow data, systemic drug uptake etc. and there is the option for interactive examination of drug deposition on a 3D VRML model of the lung mesh. In addition, all data is saved in tabulated ASCII format for direct import and manipulation in packages such as EXCEL.

Grid enabling

The EASA client is a customised interface that accepts numerical data entry from the user for the purposes of defining and submitting a Cophit job. This approach simplifies interaction with the simulation environment. Note that the purpose of the inhaled drug delivery simulation service of GEMSS is to embed the user's requirements of Cophit in parametric form, as an application residing on the EASA server. At the point of job submission, the parameters are passed from the EASA client to the EASA server hosted on the Grid client. The user has specified the properties and initial conditions for all compartments, following which the model information is assembled into a 'DEF' file, which is the input for the CFX computational fluid dynamics solver. Auxiliary text files specify the compartment properties, and the variation of input flow rate and drug mass over time. These files constitute the 'input files' and are zipped, encrypted and sent to the Grid server, which performs numerous

integrity and security checks. Note that all executable files reside on the Grid server and none are transmitted to it. Consequently, a malicious user at the EASA client has little opportunity to cause mischief since their input is tightly constrained. The Grid server performs the computationally intensive fluids solution step and post-processing, and the results files are retrieved and visualized on the client later. Because this software is used as a research tool, solution is not time-critical, unlike some of the more clinically-orientated applications. A large job might take of the order of a week to run. It is anticipated that Grid resources would be used at periods of low demand in order to reduce the cost of running the job.

Evaluation

For the end users within GEMSS (represented by ASD and IDAC), a typical respiratory simulation scenario has been constructed. The EASA application permits parametric exploration of the following problem:

“For arbitrary flow and mass fraction inhalation profiles, what is the likely deposition of particulates (of arbitrary size or composition) within the central and peripheral airways, and how might this be reflected in systemic drug uptake?”

The application has been installed on the Web server at IDAC’s headquarters in Ireland, and has been used to solve example problems on the Grid with run times from minutes to hours.

For the application developer (represented by the University of Sheffield in GEMSS) it is important to imbue confidence in the application by establishing that Cophit can provide credible solutions. Therefore, effort has been directed at numerical simulation of experimental studies performed within the Medical Physics department at Sheffield, and also scenarios discussed in the scientific literature. Three validation studies are relevant (two of them done within GEMSS), addressing numerical, experimental and clinical aspects of validation.

Numerical

The in vitro geometry of Zhang et al. (Zhang, Kleinstreuer and Kim *Aerosol Science* 2002 33:257) was assimilated within the Cophit model. Numerous simulations were run in accordance with boundary conditions specified by Zhang. Comparison of computed pressures, flows and deposition results obtained by each method, demonstrated good agreement.

Experimental

The in vitro ‘triple bifurcation’ geometry investigated by Zhang was reconstructed as a CAD file, and used to create a physical cast of the same with rapid prototyping technology. The bifurcating cast was fed with flow conditions that were simulated numerically. Outlet flows were measured and computed. Good agreement between the two was apparent.

Clinical

A group of eight adult volunteers inhaled Sodium Cromoglycate (SCG) using a characterised inhalation protocol assimilated within Cophit. Gamma scintigraphy and blood plasma measurements were used to quantify efficacy of drug delivery. The inhalation process (from device to systemic elimination) was modelled by the Cophit software and numerous simulations were run to determine predicted SCG blood plasma concentration as a function of time. Experimental and numerical data were compared, revealing satisfactory agreement.

In all cases, agreement with Cophit is encouraging. Scalability tests indicate that Cophit run time is enhanced by approximately 5-10 times with up to 16 processors, but the benefits rapidly diminish beyond this.

Feedback from industry contacts, such as Astra Zeneca, Aventis Pharma and Boehringer Ingelheim, etc. indicates that the Grid-enabled Cophit software is considered to be easy to use. Demonstration of the software generates sufficient interest that it often precipitates a request for additional features (which would require the building of modified EASA applications). A recurring appeal is for demonstrable evidence that Cophit can deliver what it claims, underlining the need for the kind of validation exercises undertaken within GEMSS, as a means of promoting confidence in the technology. The emphasis that GEMSS places on security is commended, and in general the provision of a Grid computing platform is viewed positively – provided that it is accompanied by a clear and well-defined business model.

End-user testing

The CPHIT application on the GEMSS Grid with the EASA user interface was intensively tested at ASD especially with respect to the user interface. All available examples were run, both steady-state and transient. In a time frame of several weeks extensive tests were performed at ASD considering both the simple and the complex EASA examples on the GEMSS server. They were performed to assess the performance and availability of the Grid service. IDAC also extensively tested the CPHIT application by implementing it on their EASA server and allowing ASD to participate in the testing. Tests were successful except for obvious cases when the GRID infrastructure was down for maintenance. There was some variance in the upload and download times as well. For a detailed view see the Final Evaluation and Validation report, deliverable D1.3b, and the End-user Evaluation Report, D1.3c.

Dissemination Activities

Dissemination activities have come as demonstration of Cophit at various centres, a Cophit CD and regular publications/presentations. Demonstration activities, scientific publications and presentations are summarized in section 3.8 at the end of this report.

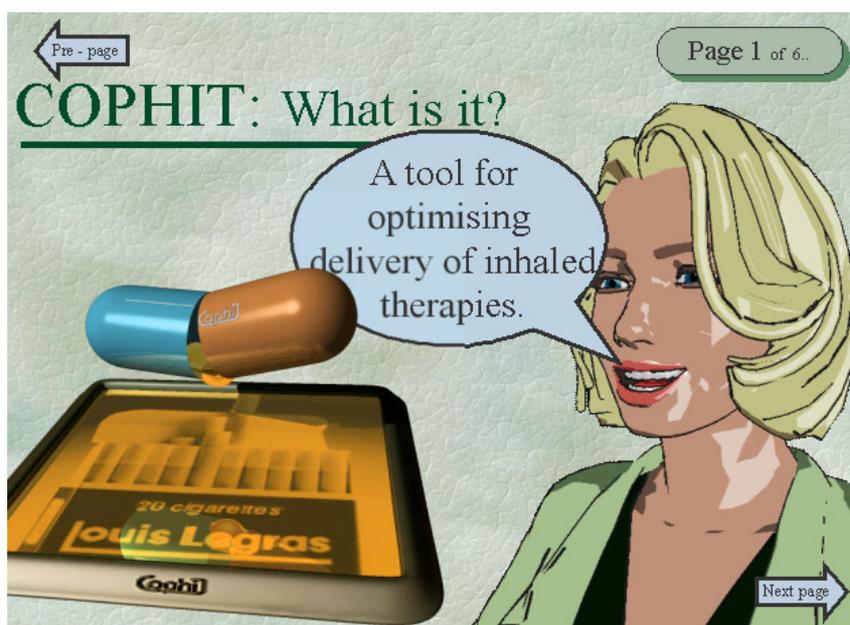


Figure 3.22: Example page from the CPHIT demo CD

Status Summary

This summary outlines key features of the GEMSS inhaled drug delivery service accomplished within the GEMSS project.

- The inhaled drug delivery service is implemented as a bespoke application negotiated between an expert developer (typically the portal provider) and the end-user
- The application has been made accessible to the end user by providing a user-friendly interface through EASA.
- The application has been partitioned into local-client and Grid-server sections, operating in conjunction with the Phase 3 middleware.
- The service uses the GEMSS security infrastructure (X.509 compliant)
- Enhanced security measures have been implemented on the Grid server to check incoming files from the portal for malicious code.
- Application development has been partially driven by industry recommendations which have dramatically altered the original GEMSS application profile. The result is an easy to use parametric application customized to the user's needs.
- The Grid enabled application fulfils the requirements specification of D1.1
- A MatLab licence is not required for any client or server system (although this is contrary to the original design specification, it resolves MatLab licensing issues)
- The documentation provided with the software release includes a tutorial guide and supplemental technical information
- A COPHIT demonstration CD including PowerPoint and html-based presentations has been developed as a means of introducing COPHIT to prospective users. It shows the steps of the solution process and demonstrates how COPHIT is used to solve inhaled drug delivery problems.
- The EASA-enabled COPHIT application is integrated with the Phase 3 middleware
- A series of extensive evaluation exercises have been undertaken and include
 - A third party running simple and complex EASA jobs
 - Validation with respect to the literature
 - Validation with respect to experimentation

Conclusion

A Grid-enabled COPHIT application is now operating successfully on the GEMSS Grid. It is apparent that large problems (i.e. ones that exceed the computational capacity of small business PC networks) can be solved securely through the computing resources provided by GEMSS. The accuracy of the simulation results is a strong function of computation time and resources, and the Grid offers a significant advantage in this respect. The latter assertion has been explored through a suitable period of evaluation. Validation exercises help to instil confidence in the ability of the Grid to deliver effective computing and the ability of the software to deliver effective and accessible respiratory simulation. The dissemination programme has included widespread contact with industry and also includes publications, conference presentations, demonstrations etc. It is only by such efforts that the profile of the Grid can be raised and the fulfillment of its promise promulgated.

Dissemination

Demonstration activities, scientific publications and presentations are summarized in section 3.8 at the end of this report.

3.4.5 Sub-task 4.5: Cardiovascular System Simulation

Application Scenario

Modelling of blood flow in arteries requires the use of sophisticated three-dimensional computational fluid dynamics (CFD) software. Using such software, flow through isolated vessel sections can be simulated to provide insight into pathologies of the heart and vasculature. However, even if the flow in only a section of the vasculature is of interest, the properties of the whole vasculature should be taken into account, because effects like peripheral vasoconstriction can have a profound impact on flow anywhere within the cardiovascular system. Unfortunately, as more of the vasculature is included within the CFD simulation, the number of vessels increases exponentially and computational prediction of the flow becomes intractable. Thus it is necessary to reduce the magnitude of the problem by encapsulating the properties of the peripheral circulation in a compartment model. In this way the problem becomes computationally tractable. Even so, transient simulation of just a small section of artery is computationally demanding, and benefits from HPC resources accessed through a grid. This application couples the full three-dimensional CFD model of a vessel section to terminating compartments and builds on principles developed in ST4.4. The software has been designed to be extensible so that new types of compartment system can be added if required. Whereas ST4.4 was EASA-driven, MatLab has been chosen for the cardiovascular application (CARDIO) because of its flexibility and its ability to cope with the sophisticated mathematical calculations required by the compartment systems.

Workflow

The specification of the three-dimensional model is performed using CFX – a commercial fluid dynamics package. The compartment software that couples to the 3D model was developed in MatLab. The CFX model is coupled to compartment systems representing the remainder of the circulatory system. The software has been implemented to have very general applicability, and it is possible for expert users to add their own compartment types. This gives great freedom in the choice of problem, as is necessary for research use or novel consultancy applications. The software is flexible, but nevertheless it has been made as user-friendly as possible through the use of a graphical user interface (written in MatLab) to set up the problems.

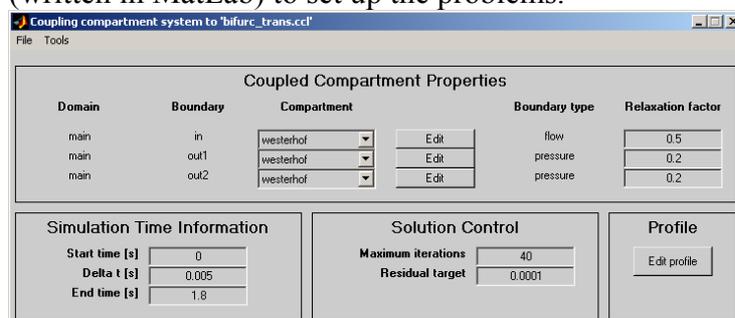


Fig. 3.23a: User interface for adding coupled compartments

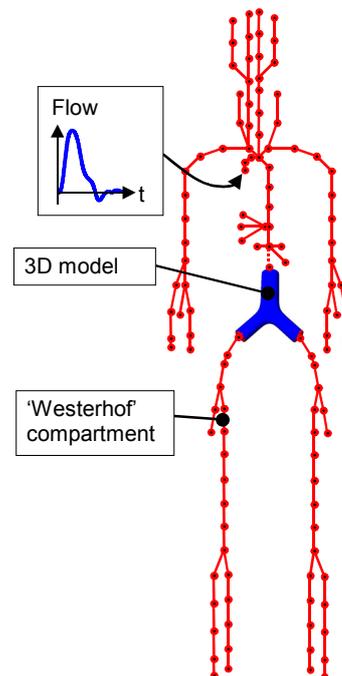


Fig. 3.23b: Example Coupled Simulation

Once the problem has been defined, input files are generated and submitted to the GEMSS client middleware, which authenticates the user to the Grid server and encrypts the input data for transmission to the Grid server. The Grid server performs the computationally intensive fluid dynamics simulation step, and solution progress can be monitored using a job

management utility. The results data is returned to the client for local visualisation, and includes both 3D flow results (Fig. 3.24b - visualised using CFX), and compartment system results (Fig. 3.24a - visualised using custom-written software).

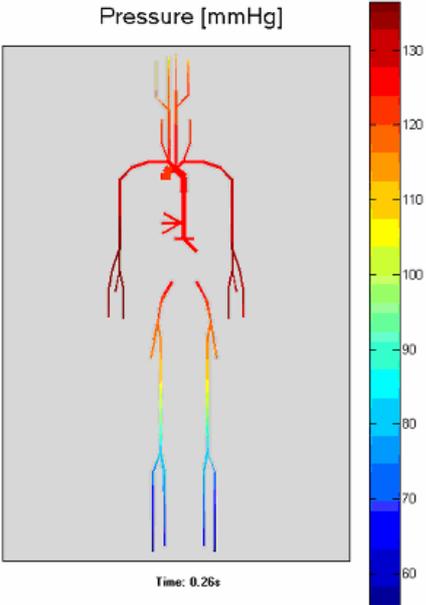


Fig. 3.24a: Compartment system results

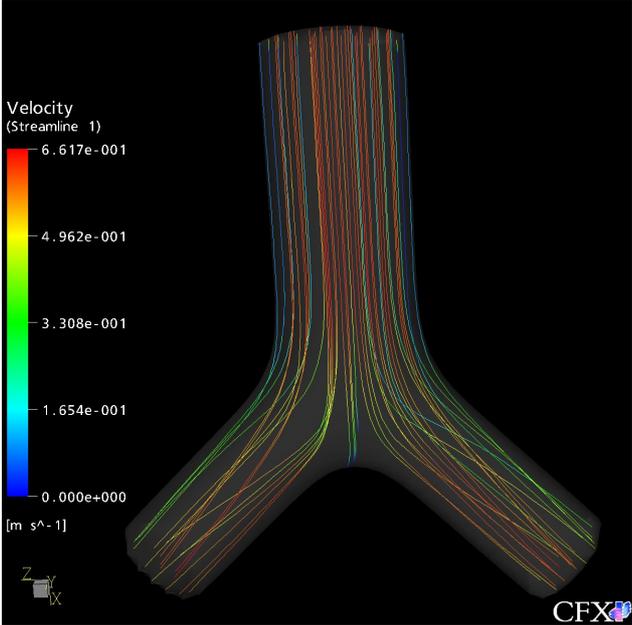


Fig. 3.24b: Flow streamlines visualised using CFX

The software has been used to model a number of real anatomical geometries, as shown in Figures 3.24c and d.

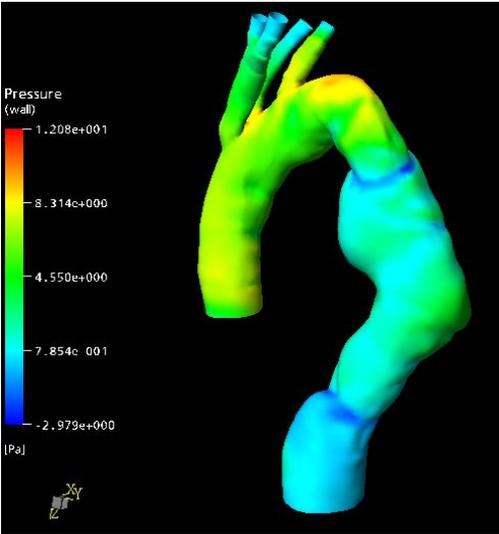


Fig. 3.24c: Pressure distribution in abnormal aortic arch

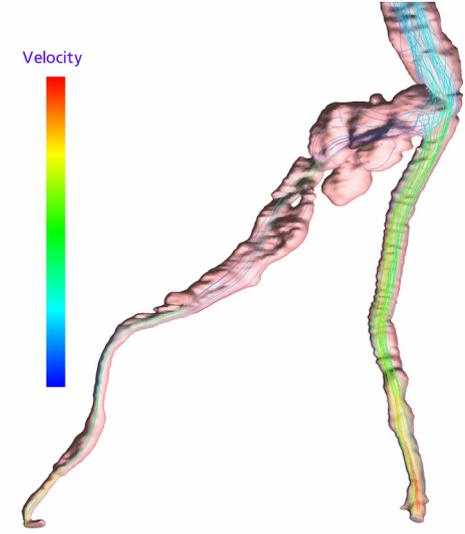


Fig. 3.24d: Flow streamlines in iliac bifurcation

Grid Enabling

The cardiovascular simulation application has been split into two parts, the client GUI and pre-processing code, and the server-side simulation code (CFX + User FORTRAN code to implement the compartment system). The server side code is installed at the service provider site. The client GUI is written in MATLAB, and this connects to the GEMSS infrastructure through a loose coupling, where calls to batch script files are made to perform grid actions (upload/start job, status enquiry, abort, and download results). The client GUI is divided into three interlinked parts – pre-processing, solution control, and post-processing. The pre-processing GUI allows the problem to be set up and then submitted for processing on the GEMSS Grid. A session file is created once a job has been uploaded so that the client does not have to remain connected for the entire duration of the job. The job-management GUI allows the users to see the job status, abort jobs, and download results. Once results have been downloaded, a post-processing GUI facilitates visualisation of both the 3D flow results and the compartment system results (see Figures 3.24a and 3.24b).

User access to the grid is controlled through the PKI infrastructure. However, in order to deal with the situation where a GEMSS account is compromised, additional checks of the application input files are performed on the GEMSS server. All executable code is pre-installed on the grid server, and so the user is denied the possibility of running arbitrary code of their choosing on the server.

For typical use of this service, compute times of up to one week would be considered acceptable. For the consultancy use of this software, computer resources would only be required occasionally, and therefore it is not cost effective for the end user to own their own HPC resource. By having access to a Grid resource, the consultancy company would be able to run more computationally demanding simulations, allowing improved simulation results.

Evaluation

The Grid-enabled cardiovascular application couples a 3D fluid dynamics solver to compartments that represent the remainder of the circulatory system. The detailed 3D model allows for detailed investigation of the flow and pressure distribution in a particular section of artery, whereas the compartment model allows global effects to be examined and influence the local 3D solution. The software allows the haemodynamic aspects of arterial disease to be investigated at both a local and a systemic scale. The evaluation phase of ST4.5 has involved the submission of hundreds of jobs with both the phase 3 and 4 clients investigating not only the capability of the Grid resource, but also the ability of the software to solve complex cardiovascular problems. In particular, the application benefits from the ability to work with 3D meshes of complex human vasculature derived from medical scan data. Effort in this area results in realistic aortic (and other) arterial meshes that add a level of anatomical relevance to the calculations not previously possible with idealized simulations.

The purpose of the compartment system is to impose physiologically realistic boundary conditions on flow through the 3D element. To this end, a flexible and sophisticated compartment system has been developed, exemplified by the ability of the software to replicate the 'compartment man' developed by Westerhof et al. (Ref. [1]). A great deal of effort has been expended on validating the behaviour of the compartment system against the literature and all results to date indicate satisfactory and robust behaviour. Thus, problems that rely on the combined 3D element and the coupled compartment system can be approached with confidence. The method has been applied to idealised geometries (for testing purposes) but has also been applied to computing the flow in the aortic arch and at the root of the mesenteric artery. This work has already been publicised in the medical scientific domain and further publications will follow.

One of the strengths of the software is its flexibility. This inevitably made the application more involved to use than the COPHIT software alone. However, the diversity of scenarios

open to the user to explore is vastly increased by this approach. The software is easily extensible: it would not be difficult to add simplified front-ends in the future for solution of specialised, parameterised problems, as with COPENIT.

Over the course of evaluation, several hundred CARDIO jobs have been submitted. This exercise has clarified the gains to be obtained by use of the Grid. Large complex models arising from anatomical geometries benefit from remote resources that a Grid service can access. Furthermore, up to a 9-fold increase in compute speed has been obtained with 16 processors. However, for this class of examples the application does not scale well beyond this number of CPUs and recruitment of further processors is less efficient. The CARDIO software is an early adopter of the phase 4 client demonstrating its successful integration with the latest GEMSS middleware release.

The CARDIO software has been developed in association with the end users represented within GEMSS (ASD and IDAC), and their comments have influenced the development process. The following issues have been highlighted:

- The software has been made as easy to install and operate as possible.
- The software has been written to allow easy addition of new types of coupled-compartment that may be required to solve novel problems.
- The software is compatible with MATLAB 5.3 – it does not require the very latest version.
- The solution step can be run locally as well as on the grid, using the same user interface. This allows approximate solutions to be obtained for a coarse mesh (and tested for convergence) before a computationally intensive high-accuracy grid run is submitted.

End-user testing

Our end users have tested the software during the formal evaluation phase. Furthermore, ASD extended the software to include a new compartment type, in close collaboration with the developer (USFD). ASD ran several example problems to test the CARDIO software. Additionally, the cardiovascular software was used to couple a CFD stenosis model of ASD to the Westerhof model to get the time-dependent velocity and pressure distribution in the artery with a stenosis. In a further step, this flow field can then be used for the CFD-based prediction of the thrombosis risk of such a stenosis. This stenosis model was also used to test the performance and availability of CARDIO on the GEMSS server. These tests were performed successfully showing a good solution stability and performance.

In summary, the developed cardiovascular software proved to be a useful tool for end-users working in the cardiovascular field. It has a very good graphical user interface which makes it easy for the end user to apply the Westerhof model to his applications and run the jobs locally or on the GEMSS Grid.

Status Summary

This summary outlines key features of the GEMSS Cardiovascular simulation service accomplished within release of deliverable D4.5.

- The cardiovascular simulation service provides coupled compartment tools for researchers or consultancy companies. These tools allow a 3D CFD model to be coupled to compartments which represent the arterial system both upstream and downstream of the model.
- The application has been partitioned into local-client and Grid-server sections.
- The Cardiovascular client interface has been implemented using MATLAB.

- The Cardiovascular software is flexible and can accommodate a wide range of flow boundary conditions peripheral to the 3D component.
- The service uses the GEMSS security infrastructure (X.509 compliant).
- Enhanced security measures have been implemented on the Grid server to check incoming files for malicious code.
- The Grid enabled application fulfils the requirements specification of D1.1.
- A MatLab licence is not required for the Grid server (although this is contrary to the original design specification, it resolves MatLab licensing issues)
- Documentation is provided with the software release and includes a tutorial guide and supplemental technical information.
- A series of extensive evaluation exercises have been undertaken and include:
 - A third party running simple and complex CARDIO jobs
 - Validation with respect to the literature

Outlook beyond the project:

The CARDIO software is already finding widespread use within the Department of Medical Physics at Sheffield, and has recently featured in several grant applications.

Conclusion

A Grid-enabled Cardiovascular application is now operating successfully on the GEMSS Grid and has been used by end-users at USFD and within GEMSS. It is apparent that large problems (i.e. ones that exceed the computational capacity of small business PC networks) can be solved securely through the computing resources provided by GEMSS. The accuracy of the simulation results is a strong function of computation time and resources, and the Grid offers a significant advantage in this respect. The evaluation period has demonstrated the efficacy of the Grid, and the ability of the software to deliver effective and accessible cardiovascular simulation. The recent release of the software has led to numerous collaborations and it will continue to be promoted through dissemination activities, highlighting the potential of the Grid for solving cardiovascular simulation problems.

Dissemination

Demonstration activities, scientific publications and presentations are summarized in section 3.8 at the end of this report.

References:

- [1] Westerhoff N., Bosman F., De Vries C.J., Noordergraaf A., Analog Studies of human systemic arterial tree, Journal of Biomechanics 1969; 2; 121-143.

3.4.6 Sub-task 4.6: Advanced Image Reconstruction

Application Scenario:

Tumour diagnosis and monitoring of metabolism are the main tasks of in vivo diagnosis in nuclear medicine by visualization of distribution of radioactive tracer in the human body. Although SPECT reconstruction suffers from low spatial resolution and poor signal-to-noise ratio compared to modern x-ray CT and MRI, it provides complimentary functional information, and is indispensable in modern clinical diagnosis. The diagnostic procedure requires the patient to receive an ionising radiation dose which provides the radiation necessary for acquisition of multiple projections by the gamma camera. The projection data is computationally reconstructed for subsequent reporting and diagnosis. A large variety of reconstruction algorithms exists, many of them based on standard filtered back-projection (FBP). This method finds extensive use in current clinical practice but it is only applicable to single slices. The modern iterative algorithms available within GEMSS offer benefits because they encompass technical and physical constraints of the imaging process and are easily extendable to 3D, but this comes at the expense of high computational effort. The Grid is well suited to the task in addition to which an implementation of image reconstruction as a Grid service could also bring access to highly sophisticated image processing resources for better diagnosis.

Workflow:

Diagnostic SPECT images are reconstructed from projection data (ie. the sum of emitted photons along a linear manifold). In practice this manifold is a cone-like sub-volume of the object, from which photons are recorded by surrounding detectors. A rectangular detector array is rotated around the patient and a series of projection data is acquired. Iterative reconstruction repeatedly modifies a postulated image matrix through comparison of pseudo-projection and measured projection data. With this method a succession of intermediate images is generated until a convergence criterion is fulfilled. The weighted contribution of each voxel of the image to a specific projection value permits accurate modelling of collimator geometry and photon scatter, and all weights for all projection values define the system matrix which characterises the system response. If N is the length of the image cube, then the number of calculations is of order N^6 for full 3D reconstruction compared to order N^4 with slice reconstruction.

Grid-enabling:

Reconstruction Kernel:

A state of the art algorithm – the OS-EM (Ordered Subsets – Maximum Likelihood) algorithm which is an advanced version of the well-known ML-EM (Maximum Likelihood – Expectation Maximization) algorithm of Shepp and Vardi [1], [2] – has been adopted to satisfy numerical and algorithmic constraints of fully 3D reconstruction and implemented. This algorithm is based on a stochastic model of Poisson distributed generation and detection of photons. Both, improved resolution and robust convergence criteria are characteristics of this algorithm.

The algorithm was implemented in ANSI-C employing a hybrid parallelization paradigm optimised for SMP-clusters. Symmetric shared memory parallelization was realised using OpenMP directives [3]. Inter-node communication was implemented using MPI from the mpich library [4].

Graphical User Interface (GUI):

The GUI (Figure 3.25) serves as a portal to the GEMSS Grid. As such it relies on the high-level GEMSS client API and provides the following functionality:

- Visualization of projection/image data
- DICOM import/export
- Reconstruction parameters
- Quality of Service support
- Image processing functionality

Implemented in Java the GUI can be launched as stand-alone application or as ImageJ plug-in. The latter enables the use of all image processing functionalities offered by ImageJ [5]. That are not only those functions included in the basic version but also every plug-in implemented with ImageJ. As ImageJ can be easily extended by new plug-ins this provides a very powerful possibility for researchers in the field of medical image processing.

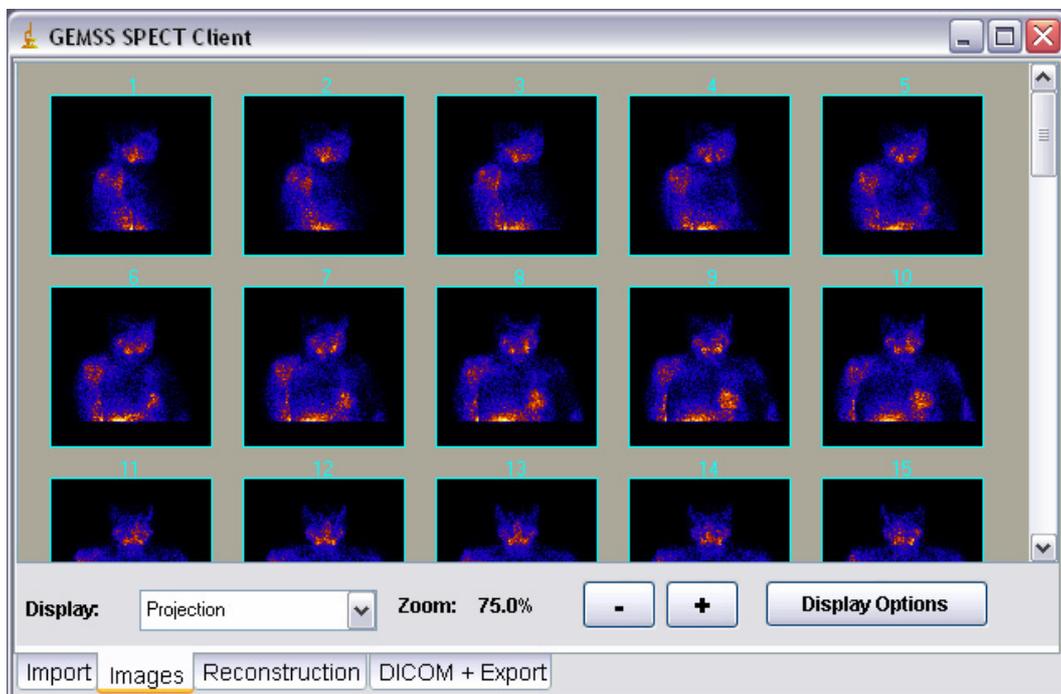


Figure 3.25: Screenshot of projection views provided by the GUI

DICOM Import/Export:

The Digital Imaging and Communications in Medicine (DICOM) standard was created by the National Electrical Manufacturers Association (NEMA) to aid the distribution and viewing of medical images [6]. Generally spoken it addresses the exchange of digital information between medical imaging equipment and other systems.

Since data compatibility with imaging modalities of different vendors is a strong criterion for the wide-spread usage of the reconstruction services it is important to provide an easy-to-use tool to import/export DICOM image and projection data. As a part of the DICOM standard the import/export of image and projection data has been implemented with the GUI.

Quality-of-Service, Performance Model:

As the actual image reconstruction takes place at some distant Grid site it is important to keep the end-users up-to-date about the progress of submitted jobs. The GUI provides information about job status (is the job still running or has it been disrupted?) and a progress bar visualizes the data provided by the GEMSS QoS module and the sophisticated performance model. This answers the question when the job will be finished.

The performance model is based on a combination of measured reference times and an analytical function to calculate the number of elements composing the system matrix of the algorithm. The analytical function applies a geometrical interpretation of the system matrix and takes into account all input parameters for a specific reconstruction.

Test Case:

The first test case does not utilise patient data but uses a phantom to allow for quantitative evaluation of the accuracy of the 3D method. Projection data from a Jaszczak phantom was reconstructed and compared to filtered back-projection (FBP). The phantom contained 600MBq Tc99m and projection data was acquired on a GE Hawkeye SPECT scanner with a 128x128 projection matrix (voxel size 4.42x4.42x4.42mm), 3 degrees rotational increment, 30 seconds acquisition time per step. Images were reconstructed using FBP with a Hanning window and compared with fully 3D OSEM reconstruction using an optimised system matrix with the alpha release software of the GEMSS project. From this phantom data the enhancement of contrast in both sections of the phantom, i.e. cold spheres and cold rods, could be shown (Figure 3.26).

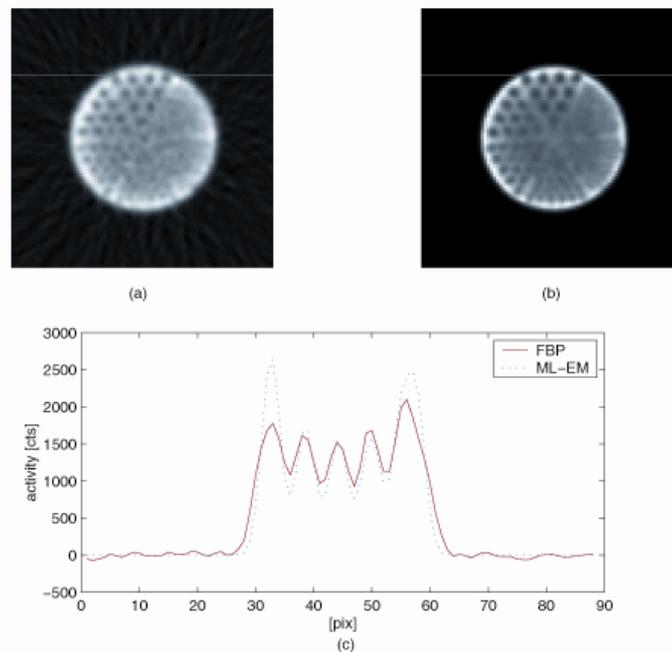


Figure 3.26: Filtered Back Projection (FBP) (a) compared to OSEM-3D (b) and profiles (c)

The second test case compares reconstructions from an I^{131} patient study of the endocrine system (projection size 64x64, 60 projections, voxel size 8.84x8.84x8.84mm).

The test data was reconstructed using the GEMSS SPECT reconstruction service. The reconstruction was performed using the fully 3D OSEM (Ordered Subsets – Maximum Likelihood) algorithm with 4 subsets and 15 iterations. For comparison reconstructed images

from standard 2D filtered back-projection (FBP) and iterative 2D reconstruction without attenuation correction (IRNC) are available.

The following figure 3.27 shows reconstructed images arranged by reconstruction method. The 3D reconstruction algorithm clearly shows better results than traditional 2D reconstruction techniques.

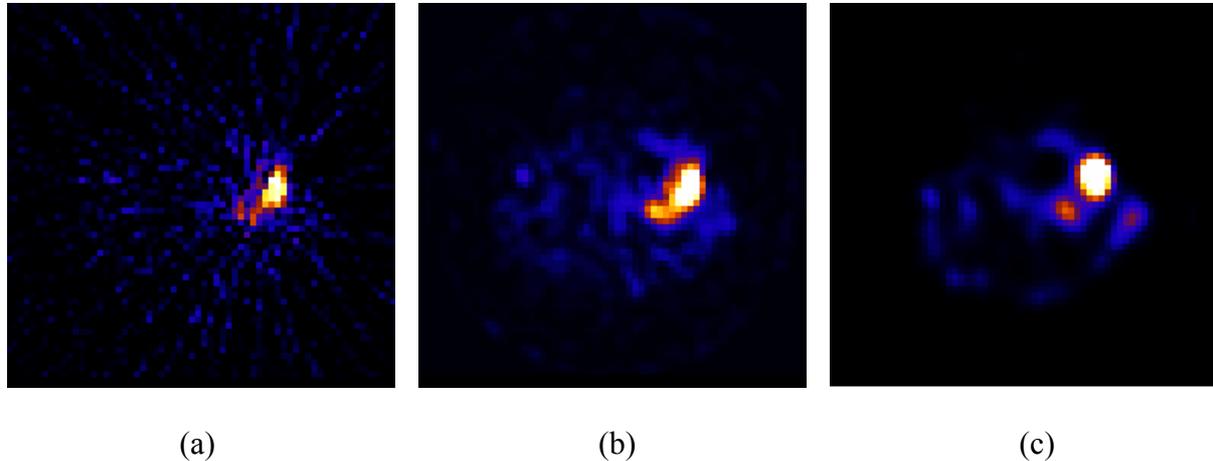


Figure 3.27: Filtered Back Projection (a) compared to IRNC (b) and GEMSS OSEM-3D (c)

Status Summary:

This summary outlines key features of the GEMSS Vienna SPECT service accomplished within this release. Within the GEMSS project, fully 3D image reconstruction was further developed from a stand-alone parallel application into a flexible Grid service, providing an easy to use, intuitive client front-end together with a fully transparent Grid-service part.

- The service uses the GEMSS security infrastructure (X.509 compliant).
- The Grid enabled application fulfils the requirements of D1.1
- The architecture of the reconstruction service was designed based on detailed user requirements and specifications, reflecting strong feasibility criteria defined by clinical users, and the trust model developed upon this information.
- The architecture reflects transparent access to GEMSS Grid resources.
- On the user front-end of the service a GUI was implemented. It provides intuitive and easy usability of the complex reconstruction service.
- Basic image processing and analysis tools are implemented into the GUI.
- The GUI is implemented as stand-alone application and as plug-in to the ImageJ biomedical software-package. This implementation guarantees easy extensibility of the functionality.
- No additional software for visualization, e.g. Matlab, Analyze of reconstruction results is necessary, and thus no license fees have to be paid.
- Easy installation enforces great acceptance from the user community.
- The reconstruction service was implemented in the GEMSS test bed, i.e. the ISS cluster in Vienna, and the NEC cluster in St. Augustin, demonstrating the realization on different hardware and security configurations.
- A distinct security policy was implemented based on the GEMSS security model.
- Data compatibility to clinical SPECT systems was achieved by implementing the industrial DICOM standard for exchange of medical image data.

- Application of flexible cost models need robust estimation of prospective runtime and necessary system resources. Reliable QoS is a fundamental basis for implementation of cost models. An accurate QoS model was developed and tested in the GEMSS testbed.
- A CD containing a demo version of the GEMSS Vienna SPECT client, a tutorial and an extended user manual, etc. has been compiled.
- A folder describing the key features of the GEMSS Vienna SPECT client has been produced for dissemination purposes.
- The results of end user evaluation will be described in D1.3c (End User Evaluation).
- Scientific publications and presentations are summarised in section 3.8.

Employing fully 3D reconstruction as a Grid service provides advanced methods of image processing to a broader medical community, benefiting from improved resolution and contrast, leading to increased sensitivity in nuclear medicine diagnosis.

Outlook beyond the project:

Further development of the GEMSS package could focus on integrated tools for real time monitoring of processes and work load distribution. Both would increase the reliability and administration of the software. Resource location tools and automated package installation tools would provide a further step towards automated administration of Software in the Grid space. For reliable use in a wider clinical context sophisticated error recovery strategies must be developed and integrated into the middleware.

Conclusion:

With the release of the GEMSS SPECT reconstruction service, fully 3D image reconstruction is accessible for a greater medical community. This meets one of the main EU R&D efforts for establishing and improving networks of experts on a European level, aided by modern IT infrastructure.

With GEMSS a framework for a secure middleware, especially addressing the issues of patient data privacy and legal issues of healthcare at an international level, was developed. Cost control is a major issue for most health services. In GEMSS billing procedures based on detailed Quality of Service models were integrated, which is a necessity for the acceptance of the reconstruction service in clinical practice.

All the application tasks within GEMSS demonstrate the development of Grid architectures from distributed data models towards workload sharing. This prospering field of Grid research is based on highly sophisticated Quality of Service models, providing accurate runtime prediction. Exactly defined performance models build the basis for a reliable end user scenario.

Beyond the scope of the GEMSS project, but as a further step towards more stability and reliability of the services, integrated tools for real time monitoring of the processes and workload should be developed. Until now only basic failure redundancy strategies are implemented, further developments of the middleware would cover this topic. Valuable end user experience should be reported after further large scale clinical field studies.

Dissemination

Demonstration activities, scientific publications and presentations are summarized in section 3.8 at the end of this report.

References:

- [1] L. Shepp and Y. Vardi. Maximum likelihood reconstruction for emission tomography. *IEEE Transactions on Medical Imaging*, 1(2): 112-122, Oct. 1982.
- [2] H.M. Hudson and R.S. Larkin. Accelerated image reconstruction using ordered subsets of projection data. *IEEE Transactions on Medical Imaging*, 13(4): 601-609, 1994.
- [3] The OpenMP Forum. OpenMP C and C++ Application Program Interface. Version 1.0, Oct. 1998. <http://www.openmp.org>
- [4] Message Passing Interface Forum. MPI: A Message Passing Interface Standard. Version 1.1, June 1995. MPI-2: Extensions to the Message Passing Interface, 1997.
- [5] ImageJ, Image Processing and Analysis in Java. <http://rsb.info.nih.gov/ij/>
- [6] DICOM – Digital Imaging and Communication in Medicine, <http://medical.nema.org/dicom/2004.html>

3.5 Workpackage 5: Exploitation, Information Dissemination and Clustering

This workpackage performed tasks related to exploitation and information dissemination. In particular it planned and co-ordinated information dissemination activities among the partners, as well as producing a post-project exploitation roadmap. A second task supported project clustering activities along two axes: generic GRID technologies and technologies for applications in the health care domain.

3.5.1 Exploitation Planning

The GEMSS consortium has broad exploitation and use intentions for the project output, covering non-commercial and commercial exploitation. The details of the GEMSS exploitation plan, documented in two separate internal deliverables – the First Exploitation Planning Report, D5.1a, and the Post Project Exploitation Plan, D5.1b, are confidential. D5.1a and D5.1b were prepared under Work Package 5 *Exploitation Planning and Information Dissemination* of the project, and complement the material in the eTIP (<http://etip.cordis.lu>) containing the Technology Implementation Plan. The D5.1a and b reports set out to describe planning of the exploitation of the results of the project. Particular attention is given to the markets in which GEMSS exploitation can take place, the opportunities within these markets, the barriers which would need to be overcome, and the planning required for the exploitation of these opportunities. The dissemination activities necessary to complement the exploitation activities are described separately in the Dissemination and Use Plan, D5.2. The exploitation planning report firstly presents a very general description of the exploitation potential of the project. These general notes are followed by the description of domain specific activities, and the description of individual partners' specific plans, and how they can be integrated for maximum benefits. An early Draft Technology Implementation Plan has been implemented using the Commission's online eTIP facility. All partners have finalized the Full Technology Implementation Plan, D5.3b. Printed versions of the public information have been submitted as deliverable D5.3a after the first project year and deliverable D5.3b after the second project year.

3.5.2 Dissemination Activities

GEMSS project partners observed current developments in the area of GEMSS activities through the attendance of conferences and events to ensure that the public was informed about the work of GEMSS and that GEMSS was aware of other projects' activities. Relevant conferences and meetings including events organized by the European Commission have been tracked in a project wide list of targeted dissemination events like international conferences, workshops, medical fairs/exhibitions and EC Concertation Meetings. Further activities include:

- **Contacts with industry**

GEMSS has established a strong focus on industrial dissemination through exhibition stands, user conferences, industrial presentations, and discussions direct with potential users.

GEMSS has links to Industry through contacts established in other projects and existing contacts especially by the industrial Consortium partners who also disseminate information about GEMSS related work to their (industrial) user

communities. For example, IDAC have been talking to 4 medical device manufacturers in the US and a number in Germany and Ireland. We have also been collaborating with a company in Japan to help them deliver their applications successfully to their customers. IDAC has been closely collaborating with CADFEM in Munich to provide internet delivered vertical applications to CADFEM's clients using EASA and potential GEMSS technologies. IDAC has also been working closely with EASA to help promote the use of EASA for GRID computing in the area of medical device applications and more general areas. The presentations from the Medical Device Seminar held in Galway, Ireland on the 23rd of January 2002 were published on the IDAC website <http://www.idacireland.com/seminars/presentations.php4>.

Another end user, ASD, has focussed dissemination activities to medical device manufacturers, the company's main customers. The technology and validated results obtained in particular with COPHIT and CARDIO have been shown to device international manufacturers of blood pumps, inhalation devices and oxygenators. Beside personal presentations, the ASD-Newsletter has informed existing and potential customers of the GEMSS technology and its potential applications in the medical device field. Also, on the ASD home page (www.asd-online.com) a link has been established to the GEMSS website to disseminate the project's results.

IDAC have been talking to 4 medical device manufacturers in the US, two of which have subsequently become customers, and a number in Germany and Ireland. We have also been collaborating with a company in Japan to help them deliver their applications successfully to their customers. IDAC have discussed the CARDIO application with some of the above companies, all of which have expressed a strong interest to learn more about it. To this end IDAC are currently looking at deploying the CARDIO application on the Internet in conjunction with MATLAB UK and the University of Sheffield, in order to better demonstrate how it might be of benefit to its customers. IDAC are also planning to talk directly to clinicians about the CARDIO tool as IDAC feels that this software has potential in the clinical environment as well as in the corporate environment. IDAC has been closely collaborating with CADFEM in Munich to provide internet delivered vertical applications to CADFEM's clients using EASA and potential GEMSS technologies. IDAC has also been working closely with EASA to help promote the use of EASA for GRID computing in the area of medical device applications and more general areas. The presentations from the Medical Device Seminar held in Galway, Ireland on the 23rd of January 2002 were published on the IDAC website:
<http://www.idacireland.com/seminars/presentations.php4>.

- **Collaboration with other projects**

GEMSS participates in the HEALTHGRID cluster formed by EU projects in the e-Health / Grid area. NEC became a member of the HEALTHGRID association.

GEMSS has established and maintained its link with the GRIDSTART project. Partner IT Innovation is a contractor of the GRIDSTART IST project. GEMSS partners chaired two GRIDSTART Technical Working Groups and took an active role.

In particular, GEMSS kept a close link to the GridLab project exchanging information, sharing experience and providing use cases.

- **Information sources**

- **Websites and Database references**

The public GEMSS website <http://www.gemss.de> was designed according to the EC DG Information Society guidelines version 1.1. It provides general information about the project. The index page offers the following links: Home, Project Details, The Consortium, Reports and Presentations.

Further material on the project is contained within a secure website, with partner access only. It provides publicity material which can be used by individual partners for their own dissemination activities.

- **TELA project database**

- http://www.dimdi.de/dynamic/de/ehealth/projekte/projekt_detail.html?pk=000309-BU&step=detail

- “Telematik-Projekt Datenbank für das deutsche Gesundheitswesen (TELA) des Deutschen Instituts für Medizinische Dokumentation und Information (DIMDI)“

- **Printings**

- GEMSS has released:

- a Project Handbook available to IST projects,
 - a Project fact Sheet,
 - a Project flyer listing exploitable results,
 - a general brochure detailing the Project,
 - general Project posters,
 - application specific posters and handouts,
 - referenced publications in scientific journals,
 - conference proceedings,
 - press releases etc. (IST Results, PraxisComputer supplement to Deutsches Ärzteblatt, Computing No 40715),
 - CD ROMs with project and application-specific informations.
 - other media articles (partner presentation, application brochure) prepared on a by-request basis.

- **Software**

- After the end of project the GEMSS middleware is available as Open Source under the LGPL license from the download section of the GEMSS web site <http://www.gemss.de>

Section 3.8 contains a concise list of scientific publications and presentations at international conferences.

3.5.3 Clustering

GEMSS participates in the HEALTHGRID cluster formed by EU projects in the e-Health / Grid area. Partner NEC is an official member of the HEALTHGRID association. GEMSS participates in the annual HEALTHGRID conferences contributing numerous presentations and posters. In addition the project contributed to a white paper on Grid for Health available on the HealthGRID web site <http://www.healthgrid.org>.

GEMSS has extended its active links with the GRIDSTART project. Partner IT Innovation is a contractor of the GRIDSTART IST project. Active support was given to various GRIDSTART activities such as EC Concertation, Technical Working Group meetings, exhibitions at IST conferences, and Grid workshops.

3.6 **Workpackage 6: Project Management**

This workpackage co-ordinated day-to-day running of the project and maintained all correspondence with the European Commission. The main goal of WP6 was to ensure the project's success by monitoring and reporting progress against goals and time scales, by establishing processes to ensure quality in project work and by anticipating and managing risk and change to the project.

3.6.1 Project Communication

The communication strategy ensured that all the Partners were fully informed about the Project status, the planning and all other issues which were important to the Partners in order to obtain maximum transparency for all involved and to increase the synergy of the co-operation. Interactive management meetings and technical meetings took an important role in the communication strategy:

- All information (like minutes of meetings, visit reports, tasks reports, relevant publications etc.) was communicated to the Project Co-ordinator, who was responsible for also channelling this information to the Partners, where appropriate.
- BASIC SUPPORT FOR COLLABORATIVE WORK (BSCW): A BSCW server has been set-up as a transparent shared work-space at the co-ordinators site. The server complements the web-server and contains all project internal documents. In addition, it serves as a common repository for documents used in preparation of deliverables. Currently 42 users from all partners are registered.
- Email reflectors have been set-up at NEC for the following (sub)groups:

All partners:	gemss@gemss.de
PMB:	pmb@gemss.de
WP1:	wp1@gemss.de
ST1.1:	st11@gemss.de
ST1.2:	st12@gemss.de
ST1.3:	st13@gemss.de
WP2:	wp2@gemss.de
ST2.1:	st21@gemss.de
ST2.2:	st22@gemss.de
WP3:	wp3@gemss.de
ST3.1:	st31@gemss.de
ST3.2:	st32@gemss.de
ST3.3:	st33@gemss.de
WP4:	wp4@gemss.de
ST4.1:	st41@gemss.de
ST4.2:	st42@gemss.de
ST4.3:	st43@gemss.de
ST4.4:	st44@gemss.de
ST4.5:	st45@gemss.de
ST4.6:	st46@gemss.de
WP5:	wp5@gemss.de

Bug report and support request tracking:

To track bug reports and support requests and automate their processing as much as possible a tracking system has been installed (roundup from <http://roundup.sourceforge.net>). Roundup is a simple-to-use and easy-to-install issue-tracking system with web, e-mail and command-line interfaces. It automatically keeps a full history of changes to issues with configurable verbosity and easy access to information about who created or last modified *any* item in the database. The system supports automatic notification and file attachments added through the web or email interfaces.

3.6.2 Management Overview

The project management has acted as contact point for all correspondence between the project and the Commission. Project-internal communication has been simplified by the provision of GEMSS mailing lists for each workpackage or subtask. All correspondence via the GEMSS lists is automatically archived. During the second year of the project, the Consortium Agreement (modified Unified Consortium Agreement) has been signed by all partners. Two Contract Amendments have been processed. Cost statements have been submitted in time and processed by the corresponding unit of the European Commission.

At least 6-monthly regular full project meetings were held during the GEMSS lifetime. Project Management Board (PMB) meetings were held during the two-day events. The project meetings were used to define and review workplan implementation details and collaborations and also to address exploitation possibilities. The regular meetings were accompanied by several technical sub-group meetings as required by the project.

The GEMSS project has successfully completed all deliverables. All central goals have been fully achieved. The work of the project has been completed within budget, lasting 30 months as expected, reflecting that both budget and schedule have been under control.

3.7 Summary and Conclusions

An innovative service oriented Grid infrastructure for the secure and lawful provision of medical application services has been successfully developed. The GEMSS Grid middleware enables distributed access to the six medical pilot services that were successfully Grid-enabled by the application partners. The final evaluation and positive response from medical end-users has shown that the technical partners have been able to respond to concerns and requirements ensuring that the users were satisfied with the final system.

A number of challenges were overcome during system integration to guarantee the successful delivery of GEMSS. The Grid middleware was successfully developed by NEC, ISS and IT INNOVATION and integrated into prototypes and the final system. Complex simulation and image processing applications were Grid-enabled and integrated. Legal issues concerning medical service provision were analysed on the European level and the outcome feed into the design of the system.

GEMSS has started at a time when Grid “standards” were changing rapidly. The project’s decision to build its own infrastructure and base it on standard web services technology proved right in the current light of the Open Grid Services Architecture and the newly announced Web Services Resource Framework. The GEMSS middleware was designed with OGSA/WS-RF in mind thus achieving abstract interoperability with leading standards.

GEMSS members have and continue to express their satisfaction with the resulting framework. Also, they have expressed their interest in continuation of the current momentum and an extension of the capabilities. The GEMSS initiative will maintain and support a testbed for at least one year after the end of the project. This not only shows the commitment of the partners but also creates explicit possibilities to further develop, disseminate and exploit the GEMSS environment.

Internal in the project medical / industrial end-user partners installed GEMSS for usage in their daily work. However, there is still a need for a wider range of applications, improved algorithms and higher functionality of the middleware to fulfill the need for medical service applications. Some of these developments are visible in the GEMSS technology demonstrators and integration with the GEMSS system is a desirable opportunity for the future.

The GEMSS project has successfully completed all deliverables. All top priority goals have been fully achieved and virtually all requirements not fully met were classified as “exploitation” requirements.

The work of the project has been completed within budget, lasting 30 months as expected, reflecting that both budget and schedule have been under control.

Overall, all central objectives have been fully achieved making GEMSS a very successful project.

3.8 Publications & Presentations

3.8.1 Publications

3.8.1.1 General

Guntram Berti, Siegfried Benkner, John W. Fenner, Jochen Fingberg, Guy Lonsdale, Stuart E. Middleton, and Mike Surridge. Medical simulation services via the Grid. In Sofie Nørager, Jean-Claude Healy, and Yves Paindaveine, editors, *Proceedings of 1st European HealthGRID Conference, Lyon, France, January 2003*, pages 248-259. EU DG Information Society, 2003.

Siegfried Benkner, Gerhard Engelbrecht, Werner Backfrieder, Guntram Berti, Jochen Fingberg, Greg Kohring, Jens Georg Schmidt, Stuart E. Middleton, David Jones, and John Fenner. Numerical simulation for eHealth: Grid-enabled medical simulation services. In G.R. Joubert, W.E. Nagel, F.J. Peters, and W.V. Walter, editors, *Parallel Computing: Software Technology, Algorithms, Architectures and Applications (Proceedings of ParCo2003, Dresden, Germany, September 2003)*, Advances in Parallel Computing. Elsevier, 2004.

David M. Jones, John W. Fenner, Guntram Berti, Frithjof Kruggel, R. A. Mehrem, Werner Backfrieder, Robert Moore, and Annette Geltmeier. The GEMSS Grid: An evolving HPC environment for medical applications. In *Proceedings of HealthGrid 2004, Clermont-Ferrand, France, January 2004*. To appear in *Methods of Information in Medicine*, 44(2), 2005.

3.8.1.2 Grid Middleware

Siegfried Benkner, Aleksander Dimitrov, Gerhard Engelbrecht, Rainer Schmidt, and Nikolay Terziev. A service oriented framework for parallel medical image reconstruction. In *Proceedings of the International Conference on Computational Science, Melbourne, Australia, June 2004*.

Siegfried Benkner, Ivona Brandic, Aleksander Dimitrov, Gerhard Engelbrecht, Rainer Schmidt, and Nikolay Terziev. Performance of java web services implementations. In *Proceedings of the 1st International Conference on Web Services*, 2003.

Junwei Cao, Guntram Berti, Jochen Fingberg, and Jens Georg Schmidt. Implementation of Grid-enabled medical simulation applications using workflow techniques. In Minglu Li, Xian-He Sun, Qianni Deng, and Jun Ni, editors, *Grid and Cooperative Computing: Second International Workshop GCC 2003 (Shanghai, China, December 2003), Part I*, volume 3032 of *LNCS*, pages 34-41. Springer Verlag, 2004.

Siegfried Benkner, Guntram Berti, Gerhard Engelbrecht, Jochen Fingberg, Greg Kohring, Stuart E. Middleton, and Rainer Schmidt. GEMSS: grid infrastructure for medical service provision. In *Proceedings of HealthGrid 2004, Clermont-Ferrand, France, January 2005*. To appear in *Methods of Information in Medicine*, 44(2), 2005.

Siegfried Benkner, Ivona Brandic, Gerhard Engelbrecht, and Rainer Schmidt. VGE - A service-oriented environment for on-demand supercomputing. In *Proceedings of the Fifth IEEE/ACM International Workshop on Grid Computing (Grid 2004)*, Pittsburgh, USA, November 2004.

Ivona Brandic, Siegfried Benkner, Gerhard Engelbrecht, and Rainer Schmidt. Towards quality of service support for grid workflows. In *Proceedings of the European Grid Conference 2005 (EGC2005)*, Amsterdam, the Netherlands, February 2005, 2005. To appear.

3.8.1.3 Legal Aspects

Jean Herveg and Yves Pouillet. *HealthGrid White Paper*, chapter Legal approaches of the HealthGrid technology. HealthGrid Consortium, 2004.

S.E. Middleton, J. Herveg, F. Crazzolaro, D. Marvin, and Y. Pouillet. GEMSS: Security and privacy for a medical grid. *Methods of Information in Medicine*, 2005. To appear.

J. Herveg and J.-M. van Gyseghem. La sous-traitance des données du patient au regard de la directive 95/46. *Lex Electronica*, 9(3), 2004. http://www.lex-electronica.org/articles/v9-3/herveg_vangyseghem.htm.

J. Herveg and J.-M. van Gyseghem. La sous-traitance des données du patient au regard de la directive 95/46. In *Proceedings of the 15th World Congress on Medical Law*, Sydney, Australia, August 2004, 2004.

Jean Herveg and Yves Pouillet. Directive 95/46 and use of GRID technologies in healthcare sector: Selected legal issues. In *Proceedings of the 1st HealthGRID Conference*, Lyon, France, January 16.-17. 2003.

3.8.1.4 Maxillofacial Surgery Planning

Guntram Berti. Image-based unstructured 3D mesh generation for medical applications. In P. Neittaanmäki, T. Rossi, K. Majava, and O. Pironneau, editors, *European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS 2004*, Jyväskylä, Finland, July 2004. University of Jyväskylä, Department of Mathematical Information Technology, 2004. CDROM.

Jens Georg Schmidt, Guntram Berti, Jochen Fingberg, Gert Wollny, and Junwei Cao. A finite-element based tool chain for the planning and simulation of maxillo-facial surgery. In P. Neittaanmäki, T. Rossi, K. Majava, and O. Pironneau, editors, *European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS 2004*, Jyväskylä, Finland, July 2004. University of Jyväskylä, Department of Mathematical Information Technology, 2004. CDROM.

Guntram Berti, Jochen Fingberg, Thomas Hierl, and Jens Georg Schmidt. An interactive planning and simulation tool for maxillo-facial surgery. In Thorsten M. Buzug and Tim C. Lueth, editors, *Perspectives in Image-guided Surgery. Proceedings of the Scientific Workshop on Medical Robotics, Navigation and Visualization (MRNV) 2004*, Remagen, Germany, March 2004, pages 311-318. World Scientific, March 11-12 2004.

Guntram Berti, Jochen Fingberg, Thomas Hierl, and Jens Georg Schmidt. Grid computing: Hochleistungs-Simulationsdienste unterstützen den Arzt. *Deutsches Ärzteblatt (PraxisComputer Supplement)*, 20(3):17-19, September 3, 2004. Cover story.

Thomas Hierl, Stephan Zachow, Gert Wollny, Guntram Berti, and Jochen Fingberg. Concepts of computer-based simulation in orthognathic surgery. *Journal of Cranio-Maxillofacial Surgery*, 32, Suppl. 1:81-82, September 2004.

Thomas Hierl, Gert Wollny, Guntram Berti, Jochen Fingberg, Jens Georg Schmidt, and Thomas Schulz. Grid-enabled medical simulation services (GEMSS) in oral & maxillofacial surgery. In *Proceedings of CURAC2004*, 2004.

Gert Wollny, Frithjof Kruggel, Thomas Hierl, and Jörg Hendriks. Assessment, validation, and visualisation of bony changes in crano-facial surgery. In *Proc of the 4th IASTED International Conference on Visualisation, Imaging, and Image Processing VIIP'04, Marbella, Spain, September 2004*, 2004.

Guntram Berti. Flexible mesh generation for segmented 2d and 3d images containing multiple materials. In *Proceedings of Remagener Physiktage 2004, Remagen, Germany, September 2004*. To appear.

3.8.1.5 Neurosurgery Support

Gert Wollny, Heiko Lippmann, Thomas Hierl, and Jörg Hendriks. Zur Vereinheitlichung und dem Vergleich nichtlinearer Registrierung. In *Proc. of Workshop Bildverarbeitung für die Medizin 2005, Heidelberg, Germany, March 2005*, Informatik Aktuell. Springer, 2005. To appear.

Gert Wollny. *Analysis of Changes in Temporal Series of Medical Images*. PhD thesis, University of Leipzig, 2003.

Heiko Lippmann and Frithjof Kruggel. Quasi-real-time neurosurgery support by MRI processing via grid computing. *Neurosurgery Clinics of North America*, 16:65-75, 2005.

Heiko Lippmann und Gert Wollny. Automatische Brain-Shift-Korrektur unter Verwendung von Grid-computing. In *Proceedings of Workshop Bildverarbeitung für die Medizin 2005, Heidelberg, Germany, March 2005*, Informatik Aktuell. Springer, 2005. To appear.

3.8.1.6 Radiosurgery Planning

J. W. Fenner, R. A. Mehrem, V. Ganesan, S. Riley, S. E. Middleton, K. Potter, and L. Walton. Radiosurgery planning supported by the GEMSS Grid. *Studies in Health Technologies and Informatics*. In press.

J. W. Fenner, R. A. Mehrem, V. Ganesan, P. Melas, and L. Walton. Practical experience of Grid-enabled health computing with the GEMSS Grid. In *Proceedings of UK e-science 'All Hands Meeting', Nottingham, UK, August 2004*, 2004. <http://www.allhands.org.uk/2004/proceedings/papers/264.pdf>.

3.8.1.7 *Inhaled Drug Delivery Simulation*

The COPHIT CD. The Interactive CDROM introduces COPHIT to prospective users through PowerPoint and html-based presentations. It shows the steps of the solution process and demonstrates how COPHIT is used to solve inhaled drug delivery problems.

3.8.1.8 *Cardiovascular System Simulation*

D. M. Jones, D. R. Hose, P. V. Lawford, D. L. Hill, R. S. Razavi, and D. C. Barber. Creation of patient-specific cfd models by morphing a previously-meshed reference geometry using image registration. In *Proceedings of Medical Image Understanding and Analysis*, pages 173-176, September 2004.

3.8.1.9 *SPECT 3D Image Reconstruction*

Martin Forster. Advanced iterative reconstruction in fully 3D SPECT. Master's thesis, TU Vienna, 2003.

W. Backfrieder, M. Forster, P. John, G. Engelbrecht, and S. Benkner. Fully 3D iterative SPECT reconstruction in a high performance computing environment. In *Proceedings of the International Conference on Mathematics and Engineering Techniques in Medicine and Biological Sciences METMBS'03, Las Vegas, USA, June 2003*, pages 216-221, 2003.

W. Backfrieder, M. Forster, G. Engelbrecht, and S. Benkner. Optimized design of VOR for 3D image reconstruction in SPECT in a service oriented parallel implementation. *Journal of Nuclear Medicine Technology*, 31(2):139, 2003.

M. Forster, S. Benkner, and W. Backfrieder. Echte 3D-Rekonstruktion in SPECT in einer netzwerkverteilten Super-Computer Umgebung. *Biomedizinische Technik*, 48(1):122-123, 2003. Gemeinsame Jahrestagung der Österreichischen, Deutschen und Schweizerischen Gesellschaft für Biomedizinische Technik BMT2003, Salzburg, Austria, September 25-27, 2003.

3.8.2 Presentations at International Conferences and Workshops

3.8.2.1 GEMSS Project Overview Presentations

Remagener Physiktage, Remagen, Germany, 25.09.2002.

Talk given by Jochen Fingberg: *Bio-numerical simulation in the SimBio and GEMSS projects.*

IST 2002 Conference, Copenhagen, 6. 11. 2002.

Invited Talk given by Guy Lonsdale: *Medical Simulation Services on the Grid.*

First HealthGrid Conference, Lyon, France, 16-17. 01. 2003.

Presentation by Guy Lonsdale: *Medical Simulation Services on the Grid.*

IDAC Ireland Medical Devices Seminar, 22.1.2004.

Presentation by Bob Moore: *Delivering Medical Applications over the Internet.*

GGF-7, Applications Update Panel (Plenary Programme), Tokyo, 5-7. 03. 2003.

Presentation by Guy Lonsdale: *Medical Services on the Grid.*

International Parallel and Distributed Processing Symposium (IPDPS 2003), Nice, France, 25. 04. 2003.

Sponsor presentation by Guy Lonsdale: *Medical Simulation Services via the Grid.*

6th HLRS Metacomputing & Grid Workshop, Stuttgart, 22-23. 5. 2003.

Invited talk given by Guy Lonsdale: *Medical Services on the Grid.*

ParCo 2003, Dresden, Germany, 3. 9. 2003.

Presentation by Jochen Fingberg: *Numerical simulation for eHealth: Grid-enabled Medical Simulation Systems.*

IST Conference Exhibition, Milan, 1.-4. 10. 2003.

Presentation of two posters on GEMSS

Presentation by Derek Sweeney: *Internet Delivery of Medical Device Simulation.*

11th CAD-FEM Users' meeting, Berlin, 14.11.2003.

Presentation by Derek Sweeney: *Internet Delivery of Medical Device Simulation Applications.*

MEDICA 2003, Düsseldorf, Germany, 19. 11. 2003.

Invited presentation by Jochen Fingberg: *Grid-enabled Medical Simulation Systems: Anwendungen für verbesserte Diagnose und Planung medizinischer Eingriffe.*

18th NEC HPC Workshop, NEC Headquarters, Tokyo, 16.12.2003

Presentation by Guy Lonsdale: *Using Grid to deliver HPC simulation to the medical community.*

2nd European Across Grid Conference & 2nd IST Concertation Meeting on Grid Research, Cyprus, 28.-29.01.2004

Poster presentation by Jochen Fingberg and Siegfried Benkner on GEMSS.

Second HealthGrid conference, Clermont-Ferrand, France, 29.-30. 1. 2004.
Poster presentation by John Fenner: *The GEMSS Grid: An Evolving HPC Environment for Medical Applications*.

Life Science research group at GGF10, Berlin, 10. 3. 2004.
Presentation by Jochen Fingberg: *Overview over the GEMSS project*.

Grid Applications in eHealth, First Results and Infrastructure Needs, eHealth concertation (EGEE/DEISA meeting), Brussels, 19. 3. 2004. Presentation by Joche Fingberg: *Overview of the GEMSS Project*.

Workshop on Web services and the Grid, organised by UNICOM, London 24.-25. 5. 2004.
Invited talk by Jochen Fingberg: *Towards secure and trusted medical simulation services*.

EC Grid Concertation Meeting, Brussels, 17. 9. 2004.
Presentation by Jochen Fingberg: *Quality of Service and Orchestration for Grid-enabled Medical Simulation Services*.

GGF-12, Life Science Grid Research Group meeting, Brussels, 22. 9. 2004.
Presentation by Guy Lonsdale: *Biomechanical modelling and treatment planning in a Grid environment*.

Remagener Physiktage, Remagen, Germany, 30.9.-2.10.2004.
Keynote lecture by Guy Lonsdale: *High Performance Computing in der Medizin*.

Supercomputing 2004, Pittsburgh, 6.-12.11.2004.
Presentation by Siegfried Benkner of 3 GEMSS posters in an exhibition booth.

12th CAD-FEM Users' meeting, Dresden, 11.11.2004.
Presentation by Derek Sweeney: *Internet Delivery of Medical Device Simulation Applications*.

IST 2004, La Hague, 15.-17.11.2004.
Presentation of GEMSS flyer by Jochen Fingberg.

International Workshop on Recent Advances in Computational Mechanics (IWACOM), Tokyo, Japan, 3.-4. 11. 2004.
Presentation by Guy Lonsdale: *Grid simulation services for the medical community*.

Seminar talk at the Institute for Biomedical Engineering and Physics, Vienna, 25.1.2005
Talk by Martin Forster: *GEMSS - Grid Enabled Medical Simulation Services*.

3.8.2.2 Presentations on Grid Middleware

European Workshop on Virtual Organizations, London, 30. 5. 2003.
Presentation given by Mike Surrige on GEMSS business models.

International Conference on Computational Science, Melbourne, Australia, 2.-4. June 2003.

S. Benkner, A. Dimitrov, G. Engelbrecht, R. Schmidt, N. Terziev: *A Service oriented framework for parallel medical image reconstruction.*

1st International Conference on Web Services, Las Vegas, USA, 23.-26. June 2003.
S. Benkner, I. Brandic, A. Dimitrov, G. Engelbrecht, R. Schmidt, N. Terziev:
Performance of Java Web Services Implementations.

Grid Resource Management Workshop, PSNC, Poznan, Poland, 20.-23. 10. 2003.
Invited talk given by Junwei Cao: *Advance Reservations of Grid Resources for GEMSS applications.*

GCC 2003, Shanghai, China, December 2003.
Talk given by Junwei Cao: *Implementation of Grid-enabled Medical Simulation Applications Using Workflow Techniques.*

Second HealthGrid conference, Clermont-Ferrand, France, 29.-30. 1. 2004.
Talk given by Gerhard Engelbrecht: *GEMSS: Grid-Infrastructure for Medical Service Provision.*

Fifth IEEE/ACM International Workshop on Grid Computing (Grid 2004), Pittsburgh, USA, November 2004.
S. Benkner, I. Brandic, G. Engelbrecht, R. Schmidt: *VGE - A Service-Oriented Environment for On-Demand Supercomputing.*

European Grid Conference, Amsterdam, February 2005.
I. Brandic, S. Benkner, G. Engelbrecht, R. Schmidt: *Towards Quality of Service Support for Grid Workflows.*

3.8.2.3 Presentations on Legal and Security Aspects

HealthGRID Conference held in Lyon, France, 16.-17. January 2003.
J. Herveg & Y. Pouillet, *Application of Directive 95/46 to the use of GRID technologies in the HealthCare Sector: selected legal issues.*

Ordre français des avocats du barreau de Bruxelles, Certificat d'aptitude à la profession d'avocat, Training, 27 May 2003.
J. Herveg, *Les fonctions spécifiques à assumer au sein de l'hôpital à raison du traitement de données à caractère personnel du patient à des fins thérapeutiques.*

HECTOR & Fédération des associations de médecins généralistes du brabant wallon, 4 October 2003.
J. Herveg, *La sous-traitance de données à caractère personnel en support à l'octroi de soins de santé. L'exemple des applications GEMSS.*

Namur, Centre de Recherches Informatique & Droit, Training, JURITIC, 20 November 2003.
J. Herveg and J.-M. van Gyseghem, *La sous-traitance de données à caractère personnel en support à l'octroi de soins de santé. L'exemple des applications GEMSS.*

Bruxelles, Symposium Telematics@health.be, 4.-5. December 2003.
J.-M. van Gyseghem, J. Herveg, L. Deplanque, M.-N. Verhaegen and Y. Pouillet,

Implications légales du réseau soins de santé, La sous-traitance de données à caractère personnel en support à l'octroi de soins de santé. L'exemple des applications GEMSS and du S3.

Ordre français des avocats du barreau de Bruxelles, Certificat d'aptitude à la profession d'avocat, Training, 15 December 2003.

J. Herveg, *La sous-traitance de données à caractère personnel en support à l'octroi de soins de santé. L'exemple des applications GEMSS.*

2nd HealthGRID Conference, France, Clermont-Ferrand, 29.-30. January 2004.

J. Herveg, *Introduction to the European legal framework regarding privacy and contractual aspects of the provision of services based on grid-technologies for medical purposes.* (Keynote speaker)

2nd HealthGRID Conference, France, Clermont-Ferrand, 29.-30. January 2004.

J. Herveg, F. Crazzolaro, S.E. Middleton, D. Marvin, Y. Pouillet (poster, + presentation by S.E. Middleton), *GEMSS: Security and Privacy for a Medical Grid.*

15th World Congress on Medical Law, Australia, Sydney, 1.-5. August 2004.

J. Herveg and J.-M. van Gyseghem, *La sous-traitance des données du patient au regard de la directive 95/46.*

Oxford University, Said Business School, United-Kingdom, Oxford, 26 January 2005.

J. Herveg, J.-M. Van Gyseghem and C. de Terwangne, *The GRID in Healthcare: Why bother about Privacy?*

3.8.2.4 Presentations on Maxillofacial surgery planning

Workshop on Medical Robotics, Navigation and Visualization (MRNV), Remagen, 11.-12. 03. 2004.

Poster presentation by Guntram Berti, Jochen Fingberg, Thomas Hierl, Jens Georg Schmidt: *An interactive planning and simulation tool for maxillo-facial surgery.*

Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, USA, 29. 3. 2004.

Presentation by Jens G. Schmidt: *A Simulation Tool for Maxillo-Facial Surgery based on FEM and AMG.*

European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS, Jyväskylä, Finland, July 2004.

Presentation by Jens Georg Schmidt: *A Finite-Element based Tool Chain for the Planning and Simulation of Maxillo-Facial Surgery.*

Presentation by Guntram Berti: *Image-based unstructured 3D mesh generation for medical applications.*

Workshop on Grid Applications Programming, Edinburgh, UK, 19.-21. 07. 2004.

Presentation by Jochen Fingberg: *Grid-enabled Medical Simulation Services in Oral & Maxillofacial Surgery.*

4th IASTED International Conference on Visualization, Imaging, and Image Processing VIIP'04, Marbella, Spain, September 2004.

Presentation by Gert Wollny: *Assessment, validation, and visualisation of bony changes in crano-facial surgery.*

Remagener Physiktage, Remagen, Germany, 30.9.-2.10.2004.

Presentation by Jens Georg Schmidt: *A finite element based toolchain for the planning and simulation of maxillo-facial surgery.*

Poster presentation by Guntram Berti: *Flexible mesh generation for segmented 2D and 3D images containing multiple materials.*

XVII European Congress for Cranio-Maxillofacial Surgery, Tours, France, September 2004.

Presentation by Thomas Hierl: *Concepts of computer-based simulation in orthognathic surgery.*

Annual meeting of Deutsche Gesellschaft für Computer-und Roboter-Assistierte Chirurgie (CURAC), Munich, Germany, 8.-9. 10. 2004.

Presentation by Thomas Hierl: *Grid-enabled Medical Simulation Services (GEMSS) in Oral & Maxillofacial Surgery.*

3.8.2.5 Presentations on Neurosurgery Planning

Workshop Bildverarbeitung für die Medizin, Heidelberg, Germany, 2005.

Gert Wollny, Heiko Lippmann, Thomas Hierl, Jörg Hendriks: *Zur Vereinheitlichung und dem Vergleich nichtlinearer Registrierung.*

Gert Wollny, Heiko Lippmann: *Automatische Brain-Shift-Korrektur unter Verwendung von Grid-computing.*

3.8.2.6 Presentations on Radiosurgery Planning

Silver Jubilee Conference of Association of Medical Physicists of India & International conference on Medical Physics (ICMP-2004), Rajiv Gandhi Cancer Institute and Research Centre, New Delhi, India, 28.-31.10.2004.

V. Ganesan, L. Walton, R. A. Mehrem, J. Fenner: *Monte Carlo Simulation for Gamma Knife Radiosurgery treatment plans using the Grid.*

UK e-science 'All Hands Meeting', Nottingham, UK, 31.8.-3.9.2004.

J. W. Fenner, R. A. Mehrem, V. Ganesan, P. Melas, L. Walton: *Practical Experience of Grid-enabled Health Computing with the GEMSS Grid.*

Annual Meeting of European Gamma Knife User Society (EGKS), Sophiahemmet (Queen Sophia Hospital) Stockholm.

V. Ganesan, L. Walton, R. A. Mehrem, J. Fenner: *Monte Carlo Simulation for Gamma Knife Radiosurgery using the 'Grid'.*

National Physics Laboratory Workshop on Monte Carlo Codes, Teddington, UK, 17.-16.3.2004.

R. Mehrem, T. Sucharov, L. Walton, J. Fenner: *Gamma Knife Radiosurgery using Monte Carlo techniques.*

12th International meeting of the Gamma knife society, Vienna, Austria, 16.-20.5.2004.

L. Walton: *APS system- Experiences and suggested further development.*

IPEM Head & Neck cancer radiotherapy conference, London, UK, 11.2.2004.
R. Mehrem, T. Sucharov, L. Walton, J. Fenner: *Gamma Knife Radiosurgery using Monte Carlo techniques.*

3.8.2.7 Presentations on Inhaled Drug Delivery Simulation

American Thoracic Society, May 2003.

E. Demoncheaux, J. Fenner, B. Brook, R. Hose, D. Bee, K. McCormack, T. W. Higenbottam: *Predictive pharmacokinetic parameters for inhaled therapies: the COPHIT approach.*

Mayneord Phillips Summer School, Oxford, UK, July 2003.

Invited talk by J. Fenner: *Modelling flow in the airways.*

European Respiratory Society, Vienna, Austria, September 2003.

E. Demoncheaux, B. Brook, J. Fenner, R. Hose et al.: *Novel paradigm for inhaled therapies: simulation of drug pharmacokinetic behaviour and effect of disease.*

Annual Congress of the European Respiratory Society, Glasgow, Scotland, UK, September 2004.

E. Demoncheaux, J. Fenner, B. Brook, R. Hose, P. Lawford, E. vanBeek, T. W. Higenbottam, K. McCormack, D. Mayer, H. U. Kauczor, S. Nichols: *Development and validation of high performance computing simulation of respiratory tract of inhaled drug and pharmacokinetics.*

Aerosol Society, Sheffield, UK, November 2004.

J. Fenner, K. Tang, Z. Varambhia, S. Nichols, B. Brook, E. Demoncheaux, K. McCormack: *Preliminary Validation of the Cophit Drug Delivery Model.*

Presentation by Ian Jones on Lung Modeling.

Presentations of COPHIT were given at the following centres:

Pfizer (R&D), Sandwich, Kent, UK

Aventis Pharma Ltd, Holmes Chapel, Cheshire, UK

Astra Zeneca, Charnwood, Leicestershire, UK

Boehringer Ingelheim GmbH, Corporate Headquarters, 55216 Ingelheim, Germany

GlaxoSmithKline, Uxbridge, Middlesex, UK

MoD DERA, Porton Down, Wiltshire, UK

MediBreathe/Cophit technical seminar (presented to industry contacts), Oxford, UK

3.8.2.8 Presentations on Cardiovascular System Simulation

21st FSI Advisory Group meeting, Dundee, Scotland, UK, November 2003.

D. R. Hose (invited speaker): *Numerical simulation of the cardiovascular system.*

J. W. Fenner: *Prediction, visualisation and validation of some clinically relevant complex flows.*

Grid Technology conference, Leeds, UK, March 2004.

D. Jones: *An Evolving HPC Environment for Medical Applications.*

11th Congress of the International Society of Rotary Blood Pumps, Bad Oeynhausen, Germany, 31.08.-02.09.2004.

Talk given by Catrin Bludszuweit: *Numerical Assessment of the Thrombosis Risk in Centrifugal Blood Pumps.*

Annual Congress European Society for Artificial Organs, Aachen, Germany, 03.09.-06.09.2004.

Talk given by Catrin Bludszuweit: *Numerical Modelling of Thermal and Mechanical Blood Damage.*

Conference Medical Image Understanding and Analysis, September 2004.

D. M. Jones, D. R. Hose, P. V. Lawford, D. L. Hill, R. S. Razavi, D. C. Barber: *Creation of patient-specific CFD models by morphing a previously-meshed reference geometry using image registration.*

3.8.2.9 Presentations on SPECT Image Reconstruction

International Conference on Mathematics and Engineering Techniques in Medicine and Biological Sciences METMBS'03, Las Vegas, Nevada, USA, June 23-26, 2003.

Talk given by Werner Backfrieder: *Fully 3D Iterative SPECT Reconstruction in a High Performance Computing Environment.*

50th Annual Meeting of the Society of Nuclear Medicine, New Orleans, Louisiana, USA, June 21-25, 2003.

Talk give by Martin Forster: *Optimized Design of VOR for 3D Image Reconstruction in SPECT in a Service Oriented Parallel Implementation.*

Gemeinsame Jahrestagung der Österreichischen, Deutschen und Schweizerischen Gesellschaft für Biomedizinische Technik BMT2003, Salzburg, Austria, September 25-27, 2003.

Talk given by Martin Forster: *Echte 3D-Rekonstruktion in SPECT in einer netzwerkverteilten Super-Computer Umgebung.*

Internal seminar talk at the Institute for Biomedical Engineering and Physics, December 16th 2003.

Talk given by Martin Forster: *Echte 3D-Rekonstruktion in SPECT in einer netzwerkverteilten Super-Computer Umgebung.*