D4.2 Software Adaptation and Testing Reports

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TABLE OF CONTENTS

LIST OF FIGURES AND TABLES

1 Executive summary

In this deliverable, which is part of our effort of adapting existing services (WP4), we report on our software adaptation work and present a range of tests that we have designed and run. This deliverable is a living document, which is periodically updated on the MAPPER wiki. The main document is a summarized and redacted version of the current wiki pages, while we provide the full Wiki content in Appendix A and B. Up to this point we provide accurate adaptation and testing reports for the four main software services within MAPPER (QosCosGrid (QCG), GridSpace, MUSCLE and AHE). Additionally, we present benchmarks of the two applications (in-stent restenosis and nanomaterials) that we demonstrated during the first review in Appendix B.

Since the start of MAPPER we have made a wide range of adaptations to integrate the four main MAPPER services. For example, AHE now supports QCG-based advance reservations while all of the MAPPER tools can conveniently be composed, launched and deployed from the GridSpace environment. In the testing reports we describe our approach to testing our component, provide a range of performance tests, and present usability surveys for the two tools that are most exposed to the user (AHE and GridSpace). Based on our performance comparisons, we find that QCG, aside from providing new functionalities, performs considerably better in many use cases than existing production middleware solutions. The surveys of AHE and GridSpace confirm that these tools provide measurable added value, and provide valuable pointers to further improve these tools. Although we provide a few performance tests of two MAPPER applications in Appendix B, a full performance assessment of the applications will be provided as part of Task 7.3.

Future versions of this deliverable will likely contain updates of the existing reports, as well as added reports for major infrastructure components that we are planning to adopt in the near future.

2 Contributors

The main contributors of this deliverable are UCL, UvA, PSNC and Cyfronet. UCL is in charge of the deliverable, and have provided the reports on AHE and the nanomaterials application. The UvA has composed the report on the in-stent restenosis, and they also worked on the reports on MUSCLE together with PSNC. PSNC in turn has provided the

reports on the QosCosGrid environment while Cyfronet has provided the reports on GridSpace.

3 Main body of the report

We present our experiences on software adaptation in section 3.1, and present our software testing approach and results in section 3.2.

3.1 Software adaptation report

3.1.1 Application-driven adaptation of QosCosGrid

The adaption of the QosCosGrid stack was driven by the acyclically-coupled and cyclically-coupled pilot MAPPER scenarios, which are comprehensively described in the Deliverable D5.2. The first scenario implied the adaptation of QosCosGrid stack to the MUSCLE environment, while the second one requested from the QCG-Broker to implement the Advance Reservation management interface. All those efforts are described in the next sections.

3.1.1.1 Adaptation for MUSCLE environment

In most parallel toolkits used within single cluster environments the master process spawns the worker processes using either SSH or local queuing/batch system native interfaces. This makes the task of exchanging contact information (e.g. listening host and port) between master and workers relatively easy as the master process is always initialized before the slave processes. With a co-allocated application this is an issue as master and workers are started independently. In the QCG stack we solved this problem by introducing the QCG-Coordinator service. The service implements two general operations: *PutProcessEntry* and *GetProcessEntry*. The master process provides contact information using the *PutProcessEntry* method, while the slave processes acquire this information using the blocking *GetProcessEntry* method. This relaxes the requirement that the kernels must be started in some particular order. The whole process of exchanging contact information is shown in Figure 1.

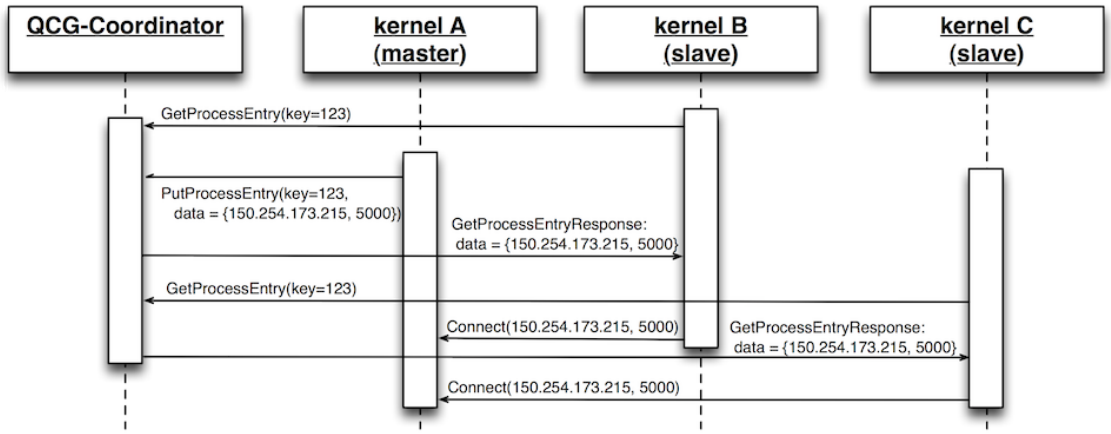


Figure 1: Contact information exchange between QCG and MUSCLE

3.1.1.2 Advance Reservation Interface

Based on the requirements of the Acyclically Coupled Multiscale Application (nanomaterials) and needs of the other MAPPER tools (GridSpace and Application Hosting Environment) the QosCosGrid stack was extended with the functionality of reserving computing resources by the users. This functionality has been added to the global service QCG-Broker, which for this purpose exploits the capabilities offered currently by the QCG-Computing services - a domain level component which provides remote access to the resources managed by queuing systems. The advance reservation of resources has been previously successfully used in the process of co-allocating MAPPER cyclically coupled parallel applications across many, heterogeneous, distributed resources. For cyclically coupled applications reservations are established by the system for the duration of a single job and automatically deleted upon its completion. For advance reservations created using the newly implemented functionality reservations are fully controlled by individual users.

Reserved resources can be later used as the containers for jobs submitted by users. QCG-Broker, in the job submission interface, accepts reservation identifiers in the two forms: global and local. The second type of identifier may be used when submitting jobs using third-party services (e.g. UNICORE in case of a cyclically coupled application in MAPPER).

The functionality of creating and managing of advance reservations has been added to the basic command-line QCG-Broker client (called QCG-Client) that offers users an access to the functionality provided by the QosCosGrid infrastructure. In addition we have developed a graphical user interface to further support the MAPPER users. We describe this portal in the next section.

3.1.1.3 Reservation Portal

The graphical user interface (GUI) is one solution to help a user to work in a complex computing environment. We developed a web-based graphical client for managing reservations via QosCosGrid. We chose a web interface because its intuitive to the user and has neglishible system requirements (users need only a reasonably up-to-date web browser). The QCG-Broker client, which has already been integrated with Vine Toolkit (http://vinetoolkit.org),has been extended in order to give users the ability to request new advance reservations and listing all already granted reservations. A screenshot of the Reservation Portal is shown in Figure 2.

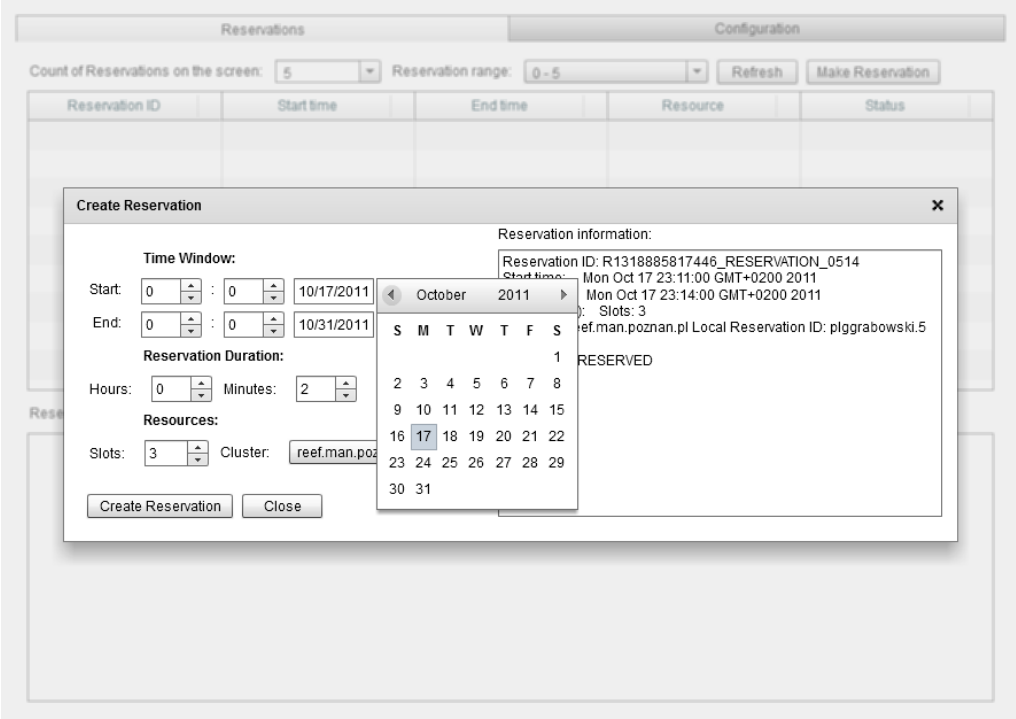


Figure 2: Screenshot of the QCG reservation portal

3.1.2 Application-driven adaptation of GridSpace

GridSpace was adapted according to multiscale application requirements gathered from the start of the project and described in D 4.1, D 8.1 and D7.1. As one of the goals of the MAPPER project is to propose a common Multiscale Modelling Language for description of multiscale applications structure, it was decided to base our tools on that language. This included:

- Developing new tools that support MML. The design of the tools was described in D 8.1 and their first prototype can be found in D 8.2. The tools present in a current prototype include Mapper Memory (MaMe) that registers submodules of multiscale applications and the relevant scale information etc. MaMe includes also MML

repository. The other new tool is Multiscale Application Designer (MAD) for composing submodules into multiscale applications. The tools were developed from stratch according to application requirements.

- Adapting GridSpace to be compatible with the new MML-based tools. This includes:
    - introducing new, infrastructure independent format of GridSpace executable experiment that can be produced from MML and additional information stored in MaMe.
    - introducing, designing and developing an interpreter-executor model of execution in Gridspace:
        - Interpreter is a software package available in the infrastructure, e.g.: Multiscale Coupling Library and Environment (MUSCLE) or Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
        - Executor is a common entity of hosts, clusters, grid brokers, etc. capable of running software that is already installed (represented as Interpreters). Examples are Application Hosting Environement (AHE) or QCG Broker

More information about inspector executor model can be found in Deliverable 8.2.

3.1.3 Application-driven adaptation of MUSCLE

MUSCLE is generally well accepted by teams that use Java for their submodels. However, MUSCLE did not support the use of MPI in its submodels, which was required for the Fusion, ISR3D, and canals applications. Technically, this is caused by the incompatibility between Java threads, which the submodels use, and MPI. Consequently, whenever someone needed MPI, they had to have the submodel start an external executable that used MPI. We adapted MUSCLE such that using MPI is now possible without the need to start executables from the submodels. Technically, when using MPI, submodels are no longer run using threads, removing the incompatibility. This change does mean that, if MPI is used, only one submodel may be run in a MUSCLE instance. This change is now being implemented in the respective applications, as it requires small changes in the application code.

Another limitation of MUSCLE was that it needed direct TCP/IP connections between the different submodels. Since high-performance machines generally have restrictive firewall settings which render direct connections impossible. We solved this problem by developing the user-space MUSCLE Transport Overlay (MTO) daemon. MTO runs on the interactive nodes of high-performance machines and relays all communication between MUSCLE submodels. This way, submodels do not communicate directly, but by help of MTO. Using the MTO is not the default, so MUSCLE still runs the same way it did before on local clusters

or computers. We present a usage example of the MTO in Figure 3. Applications do not have to adapt their code to use MTO, they only need to use the command-line flag `--intercluster` which enables the use of MTO.

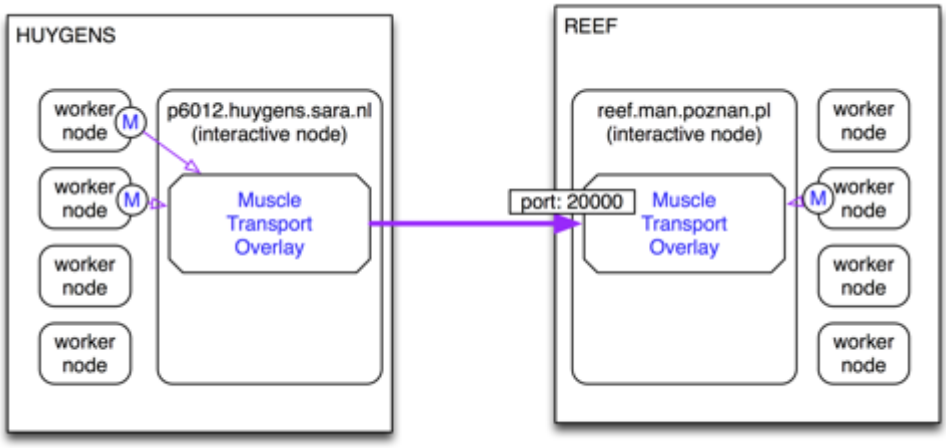


Figure 3: Overview of a distributed coupled application using MUSCLE and the MTO.

3.1.3.1 More recent adaptations

From the MUSCLE API perspective, there are now separate runtime classes for MML types such as submodels, mappers, and conduit filters. Writing the classes has been made less verbose. For instance, the scale does not need to be coded anymore but can be given as a parameter. Also conduits do not need to be initialized in the code but can be called directly by their name. Moreover, conduits can now be used in a non-blocking way.

One of the difficulties that application developers had was the lack of compatibility of MPI with MUSCLE. These compatibility issues lay in the fact that the MUSCLE core is written in Java. As a result, MUSCLE has an additional C++ interface that communicates with Java only through TCP/IP. In this way, the C++ executable does not need to be linked with Java libraries, thereby does not interfere with the low-level MPI mechanisms such as Remote Direct Memory Access. The same startup script is used so from the command-line only a "--native" flag needs to be given.

Another issue that application developers had was that some machines might not support Java (the MUSCLE core) or Ruby (the MUSCLE startup script) at all. In this case it is possible to run the MUSCLE Java on one machine, and run the C++ code the other machine. The only requirement is that the two must be able to communicate using TCP/IP.

3.1.3.2 MUSCLE 2.0

The MUSCLE development has been progressing significantly and will have its 2.0 release beginning of autumn. Its main library features are:

- A simplified Java API
- A simplified C and C++ API
- No Java or JNI required to write C++ submodels
- Added MML elements as core MUSCLE elements, including
    - Submodels
    - Fan-in and Fan-out mappers
    - Filters
    - Source and Sink
- Automatic propagation of failed submodels

The runtime features are also updated:

- Significantly reduced communication overhead
- Added features for inter-cluster communication
- Increase in throughput for inter-cluster communication by integrating MPWide, which optimises for wide-area connections.
- Compatible with MPI
- No linking between Java and C++ required
- Support for systems which are not able to run Java on their compute (worker) nodes.

Finally, the website (located at http://apps.man.poznan.pl/trac/muscle) and the documentation have been updated to include all these features.

3.1.4 Application-driven adaptation of AHE

The point of the MAPPER infrastructure is to enable the development, deployment and routine use of multiscale applications, and in that sense, all modifications made to the AHE within the scope of the MAPPER project are application driven. However, the modifications and updates that have been made to the AHE within the MAPPER project are covered in two sections. Below are described the modifications that have been made specifically to support application scenarios, and in the next section changes which have been made to facilitate communication between AHE and other tools within the MAPPER infrastructure.

3.1.4.1 Application Deployment

AHE employs the community model user workflow: expert users configure AHE with their domain knowledge concerning the grid platform being used, as well as details of the application to be executed. Once this process is complete, the expert user can share the AHE web service with the user, allowing them to perform their scientific investigations. As such, the codes which constitute the acyclically coupled application scenario developed by MAPPER in the first year were deployed on target computational resources from UCL, PL-

Grid and PRACE, and then AHE was configured to execute them. This configuration involved pointing the AHE server used by MAPPER project to submit to the QCG BES services on the target sites (described in the next section) and updating AHE application registry with details of the applications to execute.

Rather than execute an application code directly, AHE wrappers were created which launched the codes in questions and took care of the pre and post processing stages. AHE client was extended with application parsers specific to each application wrapper, designed to automate the staging of input and output data. In addition, the AHE client was modified to allow AHE to stage files that are located on a GridFTP server, as well as data from the user's local machine.

3.1.4.2 AHE 3.0

In response to the need to create more flexible simulation workflows in AHE, we have been engaged in reimplementing AHE in Java. AHE 3.0 [8] adds additional features including a workflow engine, a RESTful web service interface, a Hibernate Object Relational Mapping framework and additional enhancements to usability and reliability. The RESTful web service interface of AHE 3.0 allows the AHE server to expose its functionalities via simple operations on URIs. AHE 3.0 also incorporates a new workflow engine using JBoss's JBPM workflow engine. This allows AHE to model persistent user workflows and provides an easier mechanism to introduce more complex workflows in the future, such as error recovery, or implement additional functionalities such as SPRUCE urgent computing functionalities into AHE. Additionally, AHE 3.0 simplifies the user access to cloud resources, and attempts to bridge the gap between grid and cloud resources, making it possible for users to combine rely on both within a single application. We expect AHE 3.0 to be deployed for use by MAPPER in the final year of the project, leading to greater reliability and better performance. This is a delay compared to the term mentioned in an earlier version of this deliverable, as we prioritized bolstering the applications that use AHE over the deployment of a new version of AHE.

3.1.5 Application-driven adaptation of MPWide

The MPWide communication library for distributed computing has largely been introduced in the second year of the project, and has been adapted both to facilitate coupling of the Cerebrovascular blood flow application and to allow improved wide area communication performance within MUSCLE. We have changed the code structure to allow MPWide to be used as an entirely external library, which is now included in the HemeLB lattice-Boltzmann application. Additionally, we have developed a Python interface, which allows us to connect

the PyNS 1D blood flow simulator to MPWide, thereby establishing a channel of communication between HemeLB and PyNS.

3.1.6 Cross-tool integration efforts in QosCosGrid

The main integration effort within the first year of MAPPER in the context of the QosCosGrid middleware stack was to enable the support for submitting and monitoring jobs via the UNICORE Atomic Services (UAS, http://www.unicore.eu). The motivation for this integration is that the UNICORE services are deployed on all PRACE sites, especially the SARA Huygens system - a machine used for the demonstration during the first MAPPER Review.

QCG-Broker is a grid meta-scheduler and co-allocation service capable of submitting and managing of multi-scale jobs based on the advance reservation mechanism. To run a singe job, QCG-Broker communicates with the services providing access to the local queuing/batch systems. QCG-Broker was already also able to submit jobs via the QCG-Computing and Globus (v2.0, v4.0) services.

3.1.6.1 The UNICORE Application Programming Interface

To integrate with the UNICORE stack we exploited the Java interface of the Unicore Atomic Services (UAS) library (version 1.4.1). The API offers interfaces for communication with all services being a part of the UNICORE middleware, including: Target System Factory (TSF), Target Service System (TSS), Storage Management Service (SMS) and Registry Service.

3.1.6.2 Authorization and Authentication

UAS client library exploits "KeyStore" files to store both certificates/private keys and also Certificate Authority certificates. Because the QCG-Broker system by default stores proxy certificates delegated by user in the database, the integration with UNICORE implied implementation of an additional keystore based mechanism. In the provided by QCG-Broker solution all user certificates are stored in a single KeyStore file protected by randomly generated passwords.

3.1.6.3 The Job Description

The UNICORE system, similar to the QCG-Computing service, accepts jobs in the standardized JSDL job description format. The Executable, ApplicationName, Arguments, Environment elements are set according to the HPC-BasicProfile specification. Other job artifacts that are not covered by the JSDL standard, such as the identifier for the reservation or the earliest job start, are transmitted via the native extensions of UNICORE system.

3.1.6.4 Monitoring of Job Statuses

Because the UNICORE Atomic Services does not support notifications of job status changes (as opposed to the QCG-Computing service) the PULL mechanism has to be exploited. Thus, in order to monitor UNICORE jobs we used built-in module of QCG-Broker: "PollingManager". This module polls periodically (with the predefined time interval) about all unfinished jobs submitted to the target UNICORE system.

3.1.7 Cross-tool integration efforts in GridSpace

3.1.7.1 Introduction

We have adapted GridSpace to the MAPPER application requirements by introducing the Inspector-Executor model of execution, according to the following approach:

- We have developed a separate GridSpace Executor for each of the tool that gives access to available resources (QCG-Broker, AHE, SSH).
- We installed a GS interpreter for each software program used by MAPPER applications (e.g. MUSCLE or LAMMPS). For example, this allows MUSCLE to be run using QCG or SSH resources.

3.1.7.2 GridSpace Executor concept

GridSpace facilitates entities called executors for running scripts on remote machines. An executor is an interface that is used for accessing computational resources such as single node, job queue, web service etc. Each concrete implementation is programmed in Java so that it can be easily embedded in GridSpace application. It is also possible to call external programs when needed. More information on the Executor concept can be found in Appendix A.

3.1.7.3 Running MUSCLE from GridSpace on QCG resources

GridSpace, along with the Mapper Memory Registry (MaMe) and the Multiscale Application Designer (MAD), allows the ad-hoc composition of multiscale applications using building blocks of multiscale modelling language (MML) entities that are registered and made available for application designers. For example, MML submodules and mappers can be implemented as MUSCLE kernels. MaMe, MAD and GridSpace are able to generate MUSCLE applications as a GridSpace experiment. We also created a generic mapping of GridSpace experiments to corresponding QCG JobProfiles to enable the execution of MUSCLE applications through QCG.

3.1.7.4 GridSpace Executor for the Application Hosting Environment (AHE)

This implementation, which is under development, uses a modified AHE Client written in Java for authentication and job execution. This modified client is easily embeddable in other Java applications. The architecture of the GridSpace-AHE integration is shown in Figure 4. The AHE Executor on the GridSpace server communicates with a MyProxy server through the AHE Client and with a Stage server through the GridFTP client. The runner machine stages input from and output to the Stage server.

3.1.8 Cross-tool integration efforts in MUSCLE

As MUSCLE is meant as a low-level tool, to implement multiscale models in, no changes to MUSCLE have been made to enhance cross-tool integration. However, both QCG-Broker and Gridspace have been adapted for MUSCLE, which is listed in the respective paragraphs. One adaptation within MUSCLE itself is that the library path and class path are now possible to set as environment variables. This feature can be useful for remote execution by for instance GridSpace EW.

3.1.9 Cross-tool integration efforts in AHE

Integration between AHE and other tools in the MAPPER infrastructure happens in two directions: higher level tools are coupled to AHE to act as clients, and AHE is coupled to lower level tools, to facilitate submission. These two integration types are classified as upstream integration and downstream integration respectively, and are discussed in the sections below.

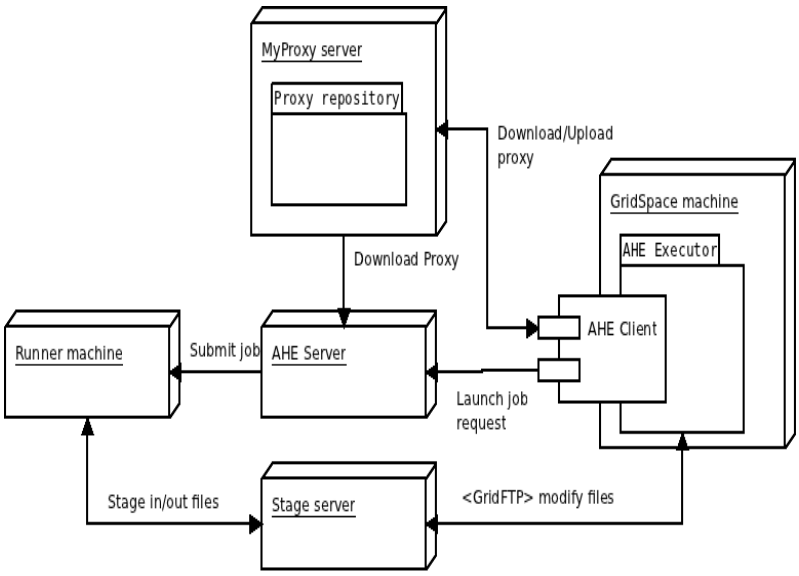


Figure 4: GridSpace and AHE integration high level architecture

3.1.9.1 Upstream Integration

Upstream integration has involved coupling AHE with GridSpace, to allow applications hosted in AHE to be called as components of a GridSpace managed workflow. Initially, this was done by preparing shell scripts which automate the launching and monitoring of an AHE hosted application, by calling AHE client commands to prepare and start the application, and then polling the application's state until it is completed. These scripts are then treated as atomic operations by GridSpace, and can be used as the building blocks of workflows.

To coupled AHE more cyclically with GridSpace, we have worked to make it possible to call the Java AHE client API directly from GridSpace. Due to compatibilities between different versions of the same library used by AHE and GridSpace, we had to update the AHE client API to use newer versions of the libraries, which involved some code refactoring. We also updated AHE client to use the Maven library loading system, in order to be further compatible with the way GridSpace worked. We also make changes to the way AHE uses proxy certificates to further enhance compatibility between AHE and GridSpace, and developed interface classes which allow the AHE to be controlled by GridSpace.

In addition to updates to the client API, we also developed generic wrapper scripts to allow GridSpace to execute arbitrary applications via AHE. GridSpace needs the ability to execute arbitrary tasks on HPC resources, for example to pre and post process data and run simulations. The generic wrappers allow GridSpace to execute any required tasks, via AHE.

3.1.9.2 Downstream Integration

The downstream integration efforts consisted of extending AHE to submit jobs via the OGF BES interface supported by QCG-Computing, now deployed on the majority of MAPPER resources. This has entailed creating a new connector to allow AHE to submit jobs to QCG-Computing, and also modifying the AHE server to enable it to stage files between sites. Previously, AHE server relied on the resource manager to perform file transfers.

Additionally, AHE has been extended to allow jobs to be submitted to into reservations created by the QCG Broker. AHE's existing advanced reservation model has been updated, entailing changes to both the client and server, to allow reservations created using QCG to pass through to QCG-Computing when jobs are submitted.

3.1.10 Cross-tool integration efforts in MPWide

The main cross-tool integration effort within MPWide is its direct integration within the MUSCLE Transport Overlay, which in turn is part of the MUSCLE 2.0 releases. Here MPWide provides automatic optimization of the wide area performance, and allows for a vastly improved throughput rate compared to the original communication kernel. At time of

writing, this integration is still in progress, but we expect MUSCLE 2.0 to be ready at the start of the third year of MAPPER.

3.2 Software testing report

3.2.1 QCG-Computing

We have measured the performance of the administrative layer component of the QosCosGrid stack: the QCG-Computing service. The benchmarking tests concerned the job submission and job management operations, which are the primary duties of any Basic Execution Service [4]. The proposed two types of the benchmarks aim to measure two important performance metrics: response time and throughput. To measure the performance benefits of QCG, we compare the performance of the QCG-Computing with a number of services that are commonly used in production infrastructures, namely gLite CREAM CE (http://grid.pd.infn.it/cream/) and UNICORE UAS (http://unicore.eu/). All the tests were performed using a benchmark program, based on the SAGA C++ API [5], which we wrote specifically for these tests.

3.2.1.1 The Testbed

The testbed consists of two systems connected with the Pionier Wide Area Network (http://www.pionier.net.pl/online/en), a client machine and the target site.

The client machine has two Intel(R) Xeon(R) CPU E5345 chips (8 cores in total), 11 GB of memory, and a round-trip time to the cluster's frontend of about 12 ms.

The target site was a the Zeus cluster in Krakow, which is part of the Polish NGI, which has about 800 nodes, ~3.000-4.000 jobs present in the system, has a scheduler poll interval of 3.5 minutes

For the purpose of the tests a subset of 8 nodes (64 cores) where assigned exclusively for the 10 user accounts used for a job submission. The benchmarked services were deployed on separate virtual machines, one of which hosts QCG-Computing and UNICORE on one virtual core and one of which hosts gLite CREAM on three virtual cores.

3.2.1.2 Benchmark 1 - Response Times

For the first benchmark we developed a program that spawns N processes (each process can use a different certificate - i.e. act as different user) that invoke the function `sustain_thread`. Next, it waits until all the running processes have ended.

Each test is characterized by: maximal number of jobs per user, number of users (concurrent processes), total number of jobs, test duration and the maximum sleep time between every

successive `query_state` call. We conducted four test sets for each of the three tested middlewares, with each of the four tests having the following parameters:

- 50 jobs x 10 users = 500 jobs, 30 minutes, SLEEP_COEF = 10 seconds,
- 100 jobs x 10 users = 1000 jobs, 30 minutes, SLEEP_COEF = 10 seconds,
- 200 jobs x 10 users = 2000 jobs, 30 minutes, SLEEP_COEF = 10 seconds,
- 400 jobs x 10 users = 4000 jobs, 30 minutes, SLEEP_COEF = 10 seconds.

3.2.1.3 Results

Test	QCG 2.0	UNICORE UAS	gLite CREAM
50	1.43	2.41	8.47
50x10	1.43	2.41	8.47
100x10	1.49	1.24 a	8.45
200x10	1.99	2.20	8.50
400x10	1.96	- b	8.24

Table 1: The average submit time of a single job. (a) indicates a test performed after the restart of the machine, caused by malfunctioning of the LUSTRE filesystem. (b) indicates executions that did not succeed.

Test	QCG 2.0	UNICORE	gLite
50x10	0.38	2.73	0.20
100x10	0.35	1.61	0.36
200x10	0.63	3.73	0.24
400x10	0.47	- b	0.21

Table 2: The average time of a query about a job status. (b) indicates executions that did not succeed.

3.2.1.4 Benchmark 2 - Throughput

The test is based on the methodology described in the paper [6]. Similar to the approach described in the paper we aimed to measure the performance from the user perspective. The test procedure consisted of two phases:

- submitting sequentially, one after another, N jobs into the target system,
- waiting until all jobs have ended.

The test job was a No OPeration (NOP) task, that finishes immediately after starting. We measured the time between the submission of the first job and the finish of the last job. We slightly improved on the test methods used in [6] by submitting the jobs using *k* processes/users, by using one client API (SAGA) instead of the command-line clients and by using a unified production environment.

The test sets were parametrized by the number of concurrent threads (*k*), whether all threads used single client certificate or not, and the total number of jobs (*N*). We present the detailed results of our throughput tests in Appendix B.

3.2.2 QCG-Broker performance metrics and tests.

We have measured several performance metrics for the QCG-Broker service, which is responsible for brokering and scheduling jobs as well as arranging reservations and co-allocation of resources. These performance metrics include:

1. submission overhead – an average time needed to serve single submission request measured as time from receiving of submission request to the passing of job to the queuing system,
2. submission throughput – measured as time needed to serve 100 submission requests,
3. reservation overhead – an average time needed to make single reservation of resources – measured as time from receiving of reservation request to creating the reservation in the queuing system,
4. reservation throughput – measured as time needed to make 100 reservations.

The main aim of comparing the times for a single request and the throughput for 100 requests is to determine the degradation of performance for a stressed system. The number of requests (100) has been chosen to stress QCG-Broker service enough, but to avoid a negative impact on underlaying systems especially queuing system managing production resources of PL-Grid infrastructure.

In spite of the fact that the analysis concern performance of QCG-Broker service, results include also elements introduced by underlying services such as QCG-Computing (remote interface to queuing system) as well as the local queuing system. The time of processing of request by these underlaying services significantly influenced the total one.

All the performance tests and measurements have been done on the production resources of PL-Grid (Polish NGI) Infrastructure - clusters: reef (PSNC), inula (PSNC), galera plus (TASK). A QCG-Broker service instance was deployed on elder7.man.poznan.pl machine – a virtual machine hosted by a physical server equipped with 2 CPUs: Intel Xeon E5345 2.33GHz and 12GB RAM with Citrix XenServer 6.0 virtualization system.

Obtained results:

1) Submission overhead:

The average time of single submission calculated for 30 requests (with 2 sec break between calls) was: 557±124 ms (α=0.05). The average time of processing by underlying services included in the given value was: 234±43 ms (α=0.05). The average time in which the service responded to the client with the job identifier (processing later the submission request in background) was: 244±50 ms (α=0.05). The brokering procedure for all requests took no more then 2 ms.

2) Submission throughput:

The time needed to submit 100 jobs was measured for 12 different numbers of threads submitting jobs (1..10, 20, 33). The average time was: 47±10 s (α=0.05).

3) Reservation overhead:

The average time of single reservation calculated for 30 requests (with 3 sec break between calls) was: 1606±633 ms (α=0.05). The average time of processing by underlaying services (included in that value) was: 1480±616 ms (α=0.05). On average 92% of time needed to reserve resources QCG-Broker waits for response mainly from the queuing system. The average time in which the service responded to the client with the reservation identifier (processing later the submission request in background) was: 132±46 ms (α=0.05).

4) Reservation throughput:

The time needed to create 100 reservation strongly depends on responsiveness of queuing system (its load and configuration of scheduler). The measurements have been done for two clusters: reef and galera. To avoid possible problems (race conditions) caused by overlapping reservation requests QCG-Broker processes reservation calls sequentially in a single thread.

a) Galera: 100 reservations was created in time: 148±3 s (α=0.05). 99% of that time QCG-Broker spent waiting for response from QCG-Computing and underlaying queuing system (the average response time for QCG-Computing (including response time from queuing system) was: 1464±688 ms (α=0.05).

b) Reef: 100 reservations was created in time: 332±40 s (α=0.05). 99% of that time QCG-Broker spent waiting for response from QCG-Computing and underlaying queuing system (the average response time for QCG-Computing (including response time from queuing system) was: 3319±15536 ms (α=0.05). For the Reef cluster there were huge differences between times of processing of single reservation call by the queuing system (min=1s, max=60s) caused by breaks in processing when the system was doing internal scheduling of jobs.

3.2.3 GridSpace

3.2.3.1 Tools Usability Tests

During first MAPPER seasonal school, we have performed usability tests of MaMe, MAD and GridSpace Experiment Workbench tools based on [7] . After making assignments (available on http://www.mapper-project.eu/web/guest/mad-mame-ew), the school participants were asked questions about usability of the system they used. The obtained average SUS score for the tools was 68 points (for 100 possible; standard deviation was 18) . The average was calculated from answers from 10 participants.

As the tools are still under the development we have also collected specific remarks that may help to improve their usability. Based on this feedback, we have proceeded to improve the interface for parameter management of application submodules. We plan to perform similar tests during the second MAPPER seasonal school planned in month 30.

3.2.3.2 GridSpace Continuous integration and testing

The GridSpace project uses continuous integration for building and testing applications to ensure that developers are constantly notified about any unexpected bugs in the codebase. The Continuum (http://continuum.apache.org) integration server builds the whole application every 4 hours. Each build consists of compiling, running unit and integration tests (see Appendix B for details) and assembling an application to a .jar or .war package. The Continuum server also deploys the latest version of the Experiment Workbench tool to a development web application server, enabling manual tests. The integration tests facilitate keeping the whole application working and detecting errors caused by changes in communication interfaces with external systems (e.g., QCG and AHE). These tests, together with the standard unit tests, ensure that existing functionality is maintained during development. To present the quality of our tests we use metrics called *code coverage* that gives a degree to which code have been tested. We present several code coverage measurements in Appendix B. We also plan to periodically perform static code analysis based only on a set of accepted code quality metrics: procedural, object-oriented and specific to the programming languages (particularly Java).

3.2.3.3 Performance, reliability and conformance tests of Experiment Workbench (EW)

As the EW is still under development we have yet to perform detailed performance, reliability and conformance tests. However, we use architecture and design patterns according to practices that will allow for carrying out such tests during the software evaluation and optimization phase. We have planned the following performance tests:

- Execute benchmark experiments in parallel through a single EW instance to examine its throughput and to estimate the hardware resource usage by a single benchmark.
- Open a number of user sessions to the same instance of Experiment Workbench to investigate the minimal resources footprint that is generated by a single user session.

In addition to that, we carry out reliability tests by monitoring the instances of EW under a real and an artificially generated load to help identify undesired long-term effects such as resource leaks.

3.2.3.4 Mapper Memory Registry (MaMe)

The MaMe is a standalone server, which uses its persistence layer in order to provide storage and publishing capabilities for a range of MAPPER use cases (module registry, XMML repository). For more details on its internal structure, please consult e.g., Section 8.2.2.3 in D8.1 deliverable.

MaMe utilizes the model-view-controller methodology for its internal architecture and, as such, need these three elements tested. We have approached to the problem threefold: by designing and applying a set of unit testing for model and controller layers, by measuring the performance of REST publishing element and by testing compatibility of the view layer with the newest web browsers. We present detailed results on this in Appendix B.

3.2.3.5 Multiscale Application Developer (MAD)

MAD is a web application providing convenient and user-friendly set of tools allowing users to compose MAPPER applications and export them to executable experiments inside GridSpace Experiment Engine. MAD relies on external components within the MAPPER infrastructure which are MaMe - the model registry and Experiment Workbench - the execution engine. MAD relies on a collection of commonly adopted libraries, which makes integration stable and require a minimal set of integration tests on the MAD side.

Testing of an interactive user interface is not easily automated. Existing web testing frameworks (e.g. Selenium) do not support recording of drag-and-drop actions. That is why the structure of the MAD project follows the MVP principles (http://code.google.com/webtoolkit/articles/mvp-architecture.html) which let unit-test user interfaces all the way up to the views. Additionally, the core of the application is abstracted into a set on controllers and presenters independent of the view engine implementation (currently GWT with supporting libraries).

3.2.4 MUSCLE

The networking code had one change, where it replaced the XDR protocol with the MessagePack protocol for serialization (http://www.msgpack.org). This makes communication between different MUSCLE instances much faster. On single instances, shared memory communication is now performed instead of TCP/IP communication. Finally, C++ to Java still uses the XDR protocol.

From these tests and the previous benchmarks, single instance communication latency shows a 20-fold decrease and throughput a 8-fold improvement. Two-instance communication latency has decreased 4-fold, while throughput has improved 10-fold. When using native code there is only a 30% increase in latency but a 12-fold decrease in throughput due to using the XDR protocol for Java-C++ communication.

The MTO software has not been significantly updated and has not been benchmarked again. It will have updated results once the integration with MPWide is fully tested

3.2.4.1 Summary of older tests

We have performed MUSCLE tests in three different environments, locally on one machine, across a local network, and across a wide area network. MUSCLE has been tested locally on a single iMac with an Intel i3 3.2 GHz processor running Mac OS X 10.7.3 to measure communication library overheads. For the local network test we connected it to a dual core Intel 2160 1.8 GHz processor running Ubuntu Server on the same network, while for the wide area test we use MTO between Reef (a PL-Grid resource in Poznan, Poland with 16 Intel Xeon E5530 cores per node) and Huygens (a PRACE machine in Amsterdam, The Netherlands; with 64 IBM Power6 cores per node).

The following measurements have been performed by sending messages of different sides from one submodel to another and back, with details in the paragraphs and tables below. Note that the average time is in fact the round-trip time (RTT), of one message being sent to the other submodel and that message returned to the first. We approximate the time for sending a single message by dividing the time for the double communication by two.

MUSCLE runs within a single instance have very high communication speeds and low latency, and the runs between two local instances also show acceptable performance, with less than 2 ms RTT and ~100 MB/s throughput. On a local network we measure a slightly higher RTT of 4 ms with ~30 MB/s throughput. Over a link between Reef and Huygens we measure a RTT of 115 ms, which is roughly three times the ping time, and a throughput

between 7 and 13 MB/sec. The limited wide area performance require further investigation, and may be caused by the connection configuration rather than the MUSCLE communication software.

Overall, MUSCLE does not seem to introduce much overhead. Largest factors are whether it is using sockets or within-process communication, and the high latency effect between distant supercomputers. We present the detailed results of our performance measurements in Appendix B.

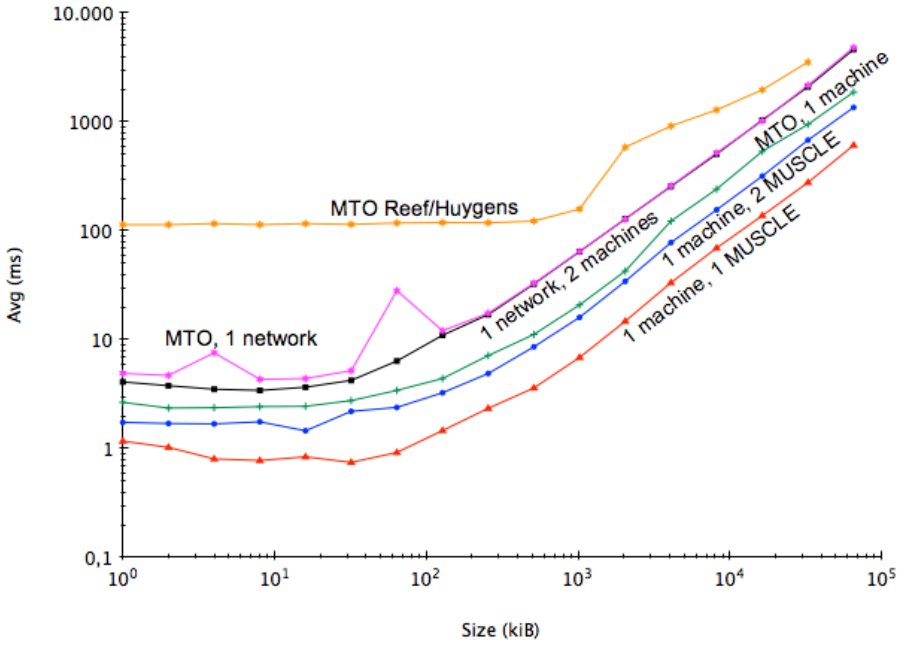


Figure 5: Network transfer timing measurements of MUSCLE across a range of networks

3.2.5 Application Hosting Environment

AHE is designed to simplify user experience, and as such benchmarking of the tool has involved conducting usability studies to compare AHE to other similar tools.

3.2.5.1 Usability Study Methodology

Here we provide a brief overview of the usability study we have performed for AHE. Further details can be found in Appendix B. We compare the AHE with both Globus and UNICORE in a variety of studies, which both are commonly used in production systems. We do this comparison to assess to what extent AHE provides added value and improved usability over the existing software in production infrastructures. Our usability study was split into two sections. In the first section participants were asked to compare Globus, UNICORE and AHE by performing three separate tasks:

- Launch an application on a grid resource using the middleware tool being tested. The application in question (pre-installed on the grid resource) sorted a list of words into alphabetical order. The user had to upload the input data from their local machine and then submit the application to the machine.
- Monitor the application launched in step 1 until complete.
- Download the output of the application back to the local machine once it has completed.

The second section compared the use of X.509 certificates to ACD (Audited Credential Delegation) authentication. In this section, users were asked to perform the following two tasks:

- Configure the AHE client with to use an X.509 certificate, and then submit a job using the graphical client.
- Authenticate to AHE using an ACD username and password, and then submit a job using the graphical client.

All of the tests ran the application on the same server, based locally in the Centre for Computational Science at University College London, which was used solely for the usability test. We invited 39 non-expert participants to the perform the usability study. Due to problems with the delivery platform, the results from six participants have been excluded, meaning that the results presented have been gathered from 33 participants.

3.2.5.2 Results

Result	Globus Toolkit	AHE CLI	UNICORE GUI	AHE GUI	AHE with Cert	AHE with ACD
Percentage of successful users	45.45	75.76	30.30	96.97	66.67	96.97
Percentage of users satisfied with tool	27.27	53.54	47.47	79.80	51.52	87.88
Percentage of users who found tool difficult to use	45.45	25.25	26.26	5.05	27.27	0.00

Table 3: Summary of statistics collected during usability trials for each tool under comparison.

Our usability tests show very clear differences between the different tools tested, based on the usability metrics defined above. Table 3 presents several key measurements from our findings. The mean times taken to complete the range of tasks with each tool are given in Figure 8. Participants able to use AHE to run their applications faster than via Globus or UNICORE, and AHE with ACD faster than AHE with X.509 certificates. We also measured

user satisfaction with the tools used. In table 3 we have summarized the percentage of participants who reported being either Satisfied or Very Satisfied with a tool.

3.2.5.3 Discussion of Results

The results presented in the previous section clearly confirm our hypotheses, that the application interaction model used by the AHE is more usable than the resource interaction model implemented in the UNICORE and Globus toolkits, with AHE found to be more usable for each of our defined usability metrics. We believe the reason for this is due to the fact that AHE hides much of the complexity of launching applications from users, meaning that (a) there are less things that can go wrong (hence the lower failure rate) and (b) there are less things for a user to remember when launching an application (hence the higher satisfaction with and lower perceived difficulty of AHE tools).

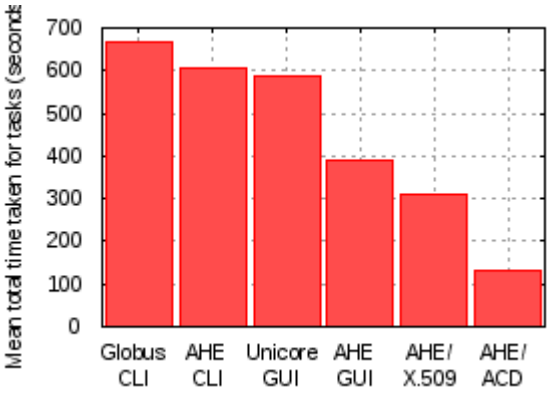


Figure 6: Mean time taken to complete a range of tasks with each tool.

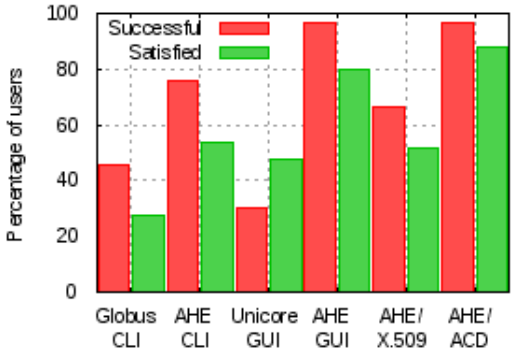


Figure 7: Comparison of the percentage of users who were satisfied with a tool and the percentage who could successfully use that tool.

3.2.6 MPWide

MPWide is currently tested as part of the HemeLB application. These tests include both unit tests, and regular functional tests. MPWide will also become part of the MUSCLE code base. We have performed a few preliminary performance tests over regular Internet using exchanges of a total size of 64MB per test, repeating each test for at least 20 times. Here we compare transfers done using MPWide with transfers that are done using the ssh-based secure copy (scp), using the 0mq communication library (http://www.zeromq.org), and using the existing communication mechanisms in MUSCLE. We summarise the results of our tests below:

Mavrino (UCL cluster, London) – Reef (PL-Grid site, Poznan):
scp: 10.7 / 16.0 MB/s (each direction respectively).
MPWide: 70 MB/s (Settings were 96 streams, 10MB/s pacing per stream, 64kB buffer size).
0mq: 30 / 110 MB/s (each direction respectively).

Reef (PL-Grid EGI site, Poznan) – Galera (PL-Grid EGI site, Gdansk):
scp: 12.8 / 21.3 MB/s (each direction respectively).
MPWide: 115 MB/s (Settings were 128 streams, 10MB/s pacing per stream, 256kB buffer size).
0mq: 64 / - MB/s (worked in one direction only).

Reef (PL-Grid EGI site, Poznan) – Huygens (PRACE Tier-1 site, Amsterdam):
scp: 32 / 9.1 MB/s (each direction respectively).
MUSCLE (older version): 18 MB/s.
MPWide: 55MB/s (Settings were 256 streams, 10 MB/s pacing per stream, 100kB buffer size).

4 Conclusions

In this deliverable we have reported on our adaptation and testing experiences of the MAPPER software. We presented a detailed account of the application-driven adaptations of QCG middleware, GridSpace, MUSCLE and AHE, and described our cross-tool integration efforts in a separate section. The QosCosGrid advance reservation feature can now be used from both AHE and GridSpace, while GridSpace has been modified to more conveniently support cyclically- and acyclically coupled multiscale models. Additionally, GridSpace now also works together with MUSCLE and AHE. A main priority in the adaptation of MUSCLE was the development of the MUSCLE Transport Overlay, which enables MUSCLE to flexibly and reliably connect submodels deployed at different locations. The AHE now supports QCG middleware, and has been adapted to allow a tighter and more robust integration with GridSpace.

We have shown that the two main MAPPER applications presented during the review maintain a good efficiency when scaled to up to 1024 cores on the Huygens supercomputer. Additionally, we find that the scaling improves for larger problem sizes. Additionally, we presented a wide range of performance and usability tests of the main MAPPER components. Among other things we have shown that the QCG middleware is more responsive than its direct competitors, and that the AHE with Audited Credential Delegation is the easiest way for non-expert users to run their applications on remote resources.

MUSCLE delivers reliable and solid performance on local sites, and reasonable performance across sites. We conclude that some of the performance limitations of MUSCLE across sites may be caused by the configuration of the underlying network and are working to resolve this. GridSpace, which is integrated with a large number of other components, features a wide range of integration, unit and code coverage tests to ensure its proper functioning when changes are made to the codebase.

In future versions of this living deliverable we aim to include updated and enhanced reports for the current components, as well as adaptation and testing reports for MAPPER services that we are planning to adopt.

5 Appendix A: Detailed software adaptation report

5.1 Application-driven adaptation of QosCosGrid

The adaption of the QosCosGrid stack was driven by the two pilot MAPPER scenarios:

- Cyclically Coupled Application Scenario,
- Acyclically Coupled Application Scenario

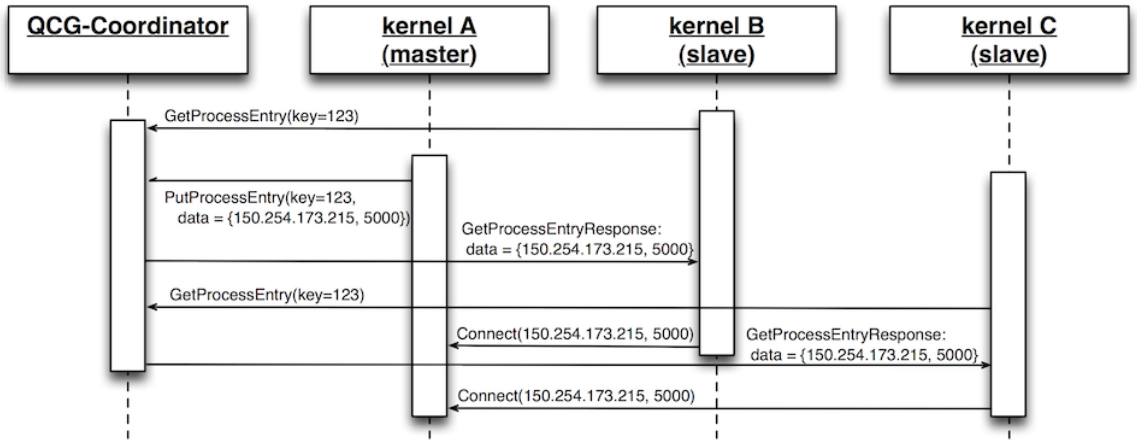
comprehensively described in the Deliverable D5.2. The first scenario implied the adaptation of QosCosGrid stack to the MUSCLE environment, while the second one requested from the QCG-Broker to implement the Advance Reservation management interface. All those efforts are described in the next sections.

5.1.1 Adaptation for MUSCLE environment

In most parallel toolkits used within single cluster environments the master process spawns the worker processes either using SSH or LRMS native interfaces. This make the task of exchanging contact information (e.g. listening host and port) between master and workers relatively easy as the master process is always initialized before the slave processes. With a co-allocated parallel application this is an issue as master and workers are started independently. In the QosCosGrid stack we solved this problem with a help of external entity: the QCG-Coordinator service. The service implements two general operations: *PutProcessEntry* and *GetProcessEntry*. The master process provides contact information using the *PutProcessEntry* method, while the slave processes acquire this information using the *GetProcessEntry* method which blocks until the information is available. This relaxes the requirement that the kernels must be started in some particular order.

- *PutProcessEntry(in: key, in: data)* - puts contact information data for a given session *key*,
- *GetProcessEntry(in: key, out: data)* - gets contact information data for a given session *key*.

The *GetProcessEntry* operation is blocking, i.e. it waits until the process data for a given *key* is available. This relaxes the requirement that the kernels must be started in some particular order. The unique session *key* is generated by QCG-Broker and distributed to all MUSCLE kernels. The whole process of exchanging contact information is shown in the below figure.



5.1.2 Advance Reservation Interface

Based on the requirements of the Cyclically Coupled Multiscale Application (nanomaterials) and needs of the other MAPPER tools (GridSpace and Application Hosting Environment) the QosCosGrid stack was extended with the functionality of reserving computing resources by the users. This functionality has been added to the global service QCG-Broker, which for this purpose exploits the capabilities offered currently by the QCG-Computing services - an domain level components which provide remote access to the resources managed by queuing systems. The Advance Reservation of resources has been previously successfully used in the process of co-allocating MAPPER cyclically coupled parallel applications into many, heterogeneous, distributed resources. The essential features that differs both cases is that for "Cyclically Coupled" applications reservations are established by the system for the duration of a single job and automatically deleted upon its completion. For advance reservation created using the newly implemented functionality reservations are fully controlled by individuall users. Users while reserving computing resources have the possibility to express their preferences providing:

- machine names to be taken into account when filtering applicable systems,
- characteristics and the amount of resources they want to reserve,

- duration of the reservation and the time window within which the reservation should be granted.

If the user was authorized for reserving resources, that means it had provided a valid definition of resource requirements and there had been free resources, the system creates a reservation and returns a globally unique identifier that uniquely identifies the reservation. For every reservation one can cancel it or query it status, which is composed of the following information:

- the description of resource requirements,
- the time when the reservation request was sent,
- the time window of the reservation,
- the reservation state and diagnostic message in case of errors.

Moreover the system returns the list of allocations (reservation on single site) created by the system with information about:

- the name of the cluster where resources have been reserved,
- the total number of reserved slots (cores),
- the local reservation identifier generated by the local batch system,
- the list of reserved worker nodes.

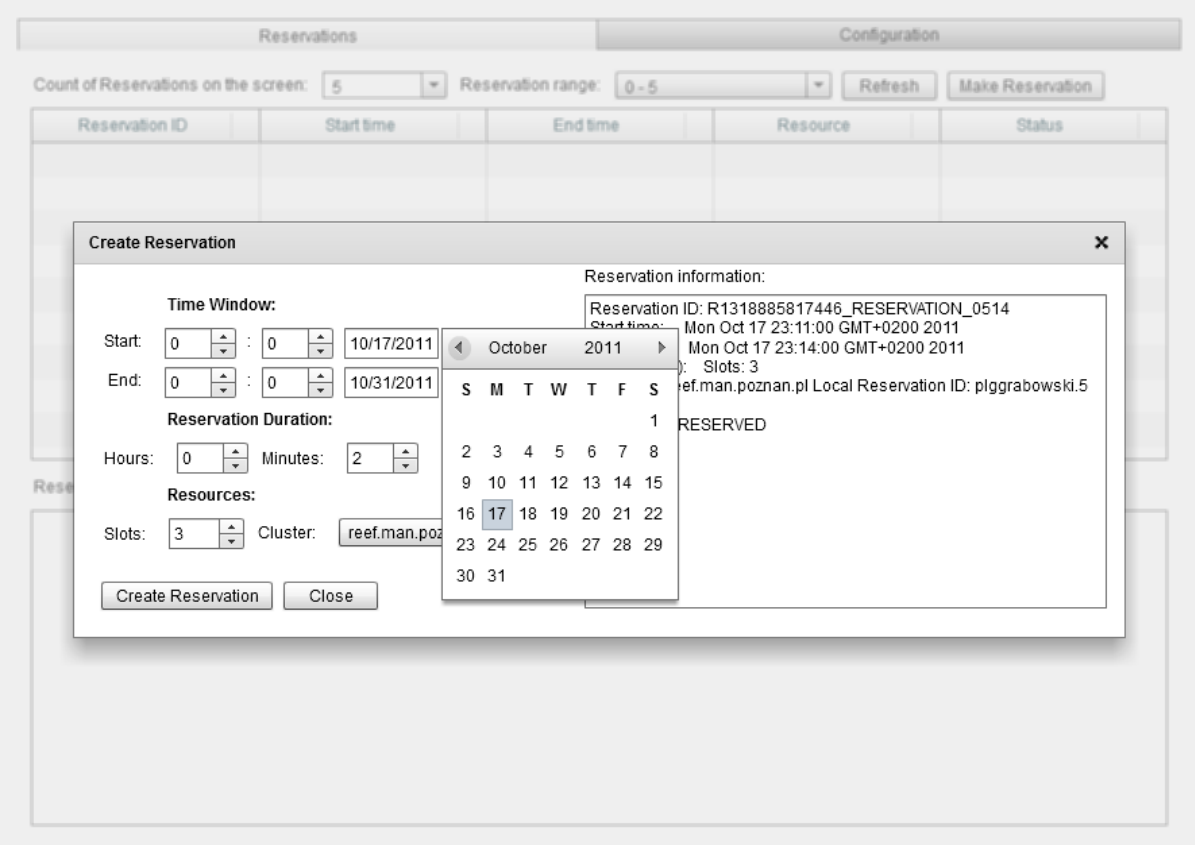
Reserved resources can be later used as the containers for jobs submitted by users. QCG-Broker, in the job submission interface, accepts reservation identifiers in the two forms: global and local. The second type of identifier may be used when submitting jobs using third-party services (e.g. UNICORE in case of a cyclically coupled application scenario).

The functionality of creating and managing of advance reservations has been added to the basic command-line QCG-Broker client (called QCG-Client) that offers users an access to the any functionality provided by the QosCosGrid infrastructure. In addition, for the convenience of the MAPPER project's users, a graphical user interface, described in the next section, was developed.

5.1.3 Reservation Portal

The use of graphical user interface (GUI) is one solution to help an user to work in a complex computing environment. In order to facilitate use of the functionality offered by the QosCosGrid services: the advance reservation of resources, we developed a Web-based graphical client for managing reservations via QosCosGrid. The Web interface was chosen for its easiness for user and almost no system requirements (the only user's requirement is a regular Web Browser). The already integrated with Vine Toolkit (http://vinetoolkit.org) the

QCG-Broker client has been extended in order to give an user the possibilities of requesting a new advance reservation and listing all already granted reservations. From the Web application it is also possible to cancel the reservation previously created. The portal was implemented in the Adobe Flash (Flex) technology, thus minimizing the risk of malformed application layout related to the lack of full compliance of current web browsers with the standards. The reservation portlet was embedded into the portal that supports nanotechnology scientific computing http://nano.man.poznan.pl. The screenshot of the Reservation Portal is presented in the below figure.



5.2 Application-driven adaptation of GridSpace

GridSpace was adapted according to multiscale application requirements gathered from the very beginning of the project and described in D 4.1, D 8.1 and D7.1. As one of the goals of the MAPPER project is to propose a common Multiscale Modelling Language for description of multiscale applications structure, it was decided to base our tools on that language. This included:

- developing new tools that support MML. The design of the tools was described in D 8.1 and their first prototype can be found in D 8.2. The tools present in a current prototype include Mapper Memory (MaMe) that registers submodules of multiscale

applications and the relevant scale information etc. MaMe includes also MML repository. The other new tool is Multiscale Application Designer (MAD) for composing submodules into multiscale applications. The tools were developed from stratch according to application requirements.

- adapting GridSpace to be compatible with the new MML-based tools. This included:
    - introducing new, infrastructure independent format of GridSpace executable experiment that can be produced from MML and additional information stored in MaMe.
    - introducing, designing and development of interpreter-executor model of execution in Gridspace:
        - Interpreter is a software package available in the infrastructure, e.g.: Multiscale Coupling Library and Environment (MUSCLE) or Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
        - Executor is a common entity of hosts, clusters, grid brokers, etc. capable of running software that is already installed (represented as Interpreters). Examples are Application Hosting Environement (AHE) or QCG Broker

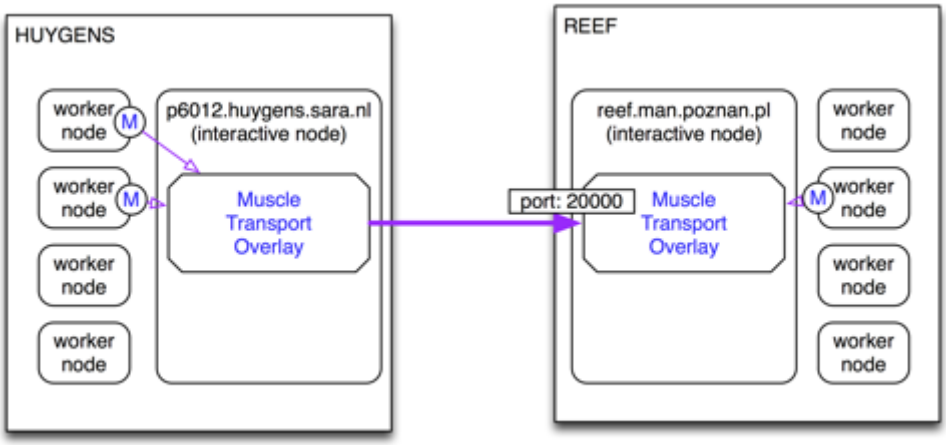
More information about inspector executor model can be found in D 8.2. Next section describes how we have used inspector-executor model in cross-tool integration.

5.3 Application-driven adaptation of MUSCLE

By teams that use Java for their submodels, MUSCLE was generally well accepted. However, MUSCLE did not support the use of MPI in its submodels, which was required from at least the Fusion, ISR3D, and canals applications. Technically, this is caused by the incompatibility between Java threads, which the submodels use, and MPI. Consequently, whenever someone needed MPI, they had to have the submodel start an external executable that used MPI. By adapting MUSCLE, using MPI is now possible within MUSCLE, without the need to start executables from submodels. Technically, when using MPI, submodels are not run in a Thread anymore, removing the incompatibility. This change does mean that only one submodel may be run in a MUSCLE instance, if it wants to use MPI. This change is now being implemented in the respective applications, as it requires small changes in their code.

Another limitation of MUSCLE, discovered by trying to do distributed multiscale computing on high-performance machines, was that it needed direct TCP/IP communication between the different submodels. Since high-performance machines generally have restrictive firewall settings, this was not possible in this setting. The problem was solved by implementing the user-space MUSCLE transport overlay daemon (MTO). MTO runs on the interactive nodes of

high-performance machines and relays all communication between MUSCLE submodels. This way, submodels do not communicate directly, but by help of MTO. Using the MTO is not the default, so MUSCLE still runs the same way it did before on local clusters or computers. The use of MTO is graphically displayed in the following figure.



Applications do not have to adapt their code to use MTO, they only need to use the command-line flag `--intercluster` which enables the use of MTO.

5.4 Application-driven adaptation of AHE

The point of the MAPPER infrastructure is to enable the development, deployment and routine use of multiscale applications, and in that sense, all modifications made to the AHE within the scope of the MAPPER project are application driven. However, the modifications and updates that have been made to the AHE within the MAPPER project are covered in two sections. Below are described the modifications that have been made specifically to support application scenarios, and in the next section changes which have been made to facilitate communication between AHE and other tools within the MAPPER infrastructure.

5.4.1 Application Deployment

AHE employs the community model user workflow: expert users configure AHE with their domain knowledge concerning the grid platform being used, as well as details of the application to be executed. Once this process is complete, the expert user can share the AHE web service with the user, allowing them to perform their scientific investigations. As such, the codes which constitute the acyclically coupled application scenario developed by MAPPER in the first year were deployed on target computational resources from UCL, PL-Grid and PRACE, and then AHE was configured to execute them. This configuration involved pointing the AHE server used by MAPPER project to submit to the QCG BES services on the

target sites (described in the next section) and updating AHE application registry with details of the applications to execute.

Rather than execute an application code directly, AHE wrappers were created which launched the codes in questions and took care of the pre and post processing stages. AHE client was extended with application parsers specific to each application wrapper, designed to automate the staging of input and output data. In addition, AHE client was modified to allow AHE to stage files that are located on a GridFTP server, as well as data from the user's local machine.

5.4.2 AHE 3.0

In response to the need to create more flexible simulation workflows in AHE, we have been engaged in reimplementing AHE in Java. AHE 3.0 adds additional features including a workflow engine, a RESTful web service interface, a Hibernate Object Relational Mapping framework and additional enhancements to usability and reliability. The RESTful web service interface of AHE 3.0 allows the AHE server to expose its functionalities via simple operations on URIs. AHE 3.0 also incorporates a new workflow engine using JBoss's JBPM workflow engine. This allows AHE to model persistent user workflows and provides an easier mechanism to introduce more complex workflows in the future, such as error recovery, or implement additional functionalities such as SPRUCE urgent computing functionalities into AHE. With the re-implementation complete, we expect AHE3.0 to be deployed for use by MAPPER in the second year of the project, leading to greater reliability and better performance.

5.5 Cross-tool integration efforts in QosCosGrid

The main integration effort within the first year of MAPPER project in the context of the QosCosGrid middleware stack was to enable the support for submitting and monitoring jobs via the UNICORE Atomic Services (UAS)[footnote:[http://unicore.eu/].] The motivation for this integration was the fact that the UNICORE services are deployed on all PRACE sites, especially the SARA Huygens system - a machine used for the demonstration during the first MAPPER Review.

QCG-Broker is a grid meta-scheduler and co-allocation service capable of submitting and managing of multi-scale jobs basing on the advance reservation mechanism. In order to run a singe job, QCG-Broker communicates with the services providing an access to the Local Resource Management Systems (so called batch systems). Before the MAPPER project QCG-Broker was capable of submitting jobs via the QCG-Computing and Globus (v2.0, v4.0) services.

5.5.1 The UNICORE Application Programming Interface

To integrate with the UNICORE stack we exploited the Java interface of the Unicore Atomic Services (UAS) library (version 1.4.1). The API offers interfaces for communication with all services being a part of the UNICORE middleware, including: Target System Factory (TSF), Target Service System (TSS), Storage Management Service (SMS) and Registry Service.

5.5.2 Authorization and Authentication

UAS client library exploits "KeyStore" files to store both certificates/private keys and also Certificate Authority certificates. Because the QCG-Broker system by default stores proxy certificates delegated by user in the database, the integration with UNICORE implied implementation of an additional keystore based mechanism. In the provided by QCG-Broker solution all user certificates are stored in a single KeyStore file protected by randomly generated passwords.

5.5.3 The Job Description

The UNICORE system, similar to the QCG-Computing service, accepts jobs in the standardized JSDL job description format. The Executable, ApplicationName, Arguments, Environment elements are set according to the HPC-BasicProfile specification. Other job artifacts, that are not covered by the JSDL standard, such as the identifier for the reservation or the earliest job start, are transmitted via the native extensions of UNICORE system.

5.5.4 Monitoring of Job Statuses

Because the UNICORE Atomic Services does not support notifications of job status changes (as opposed to the QCG-Computing service) the PULL mechanism has to be exploited. Thus, in order to monitor UNICORE jobs we used built-in module of QCG-Broker: "PollingManager". This module polls periodically (with the predefined time interval) about all unfinished jobs submitted to the target UNICORE system.

5.6 Cross-tool integration efforts in GridSpace

5.6.1 Introduction

As described in a previous section, we have adapted GridSpace to MAPPER application requirements by introducing Inspector - Executor model of execution. The integration of GridSpace with other MAPPER tools we have used following approach.

- For each of the tool that give access to available resources (QCG, AHE, SSH) we have developed separated GridSpace Executor
- Each software used by MAPPER applications (e.g. MUSCLE or LAMMPS) was installed as one of GridSpace interpreters. In particular, MUSCLE can currently be run using QCG or SSH resources.

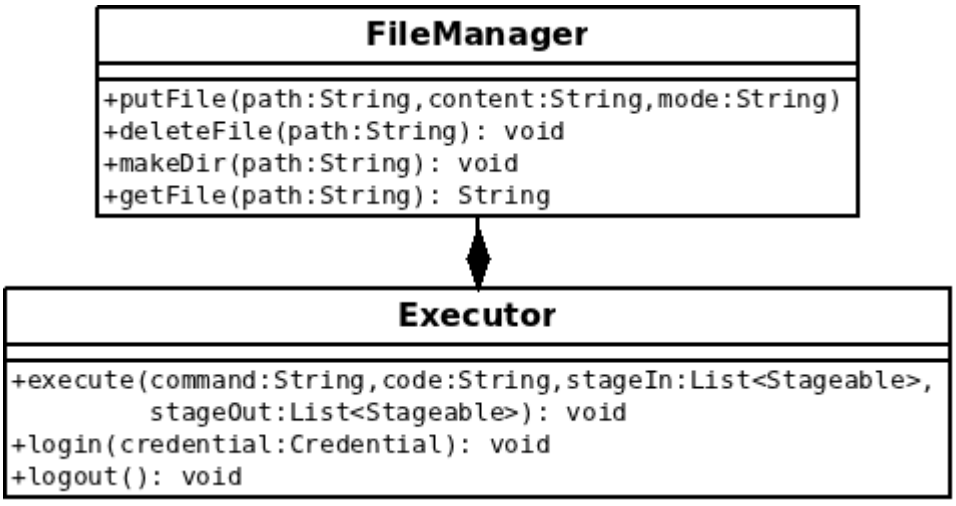
GridSpace Executor concept

GridSpace facilitates entities called executors for running scripts on remote machines. An executor is an interface that is used for accessing computational resources such as single node, job queue, web service etc. Each concrete implementation is programmed in Java so that it can be easily embedded in GridSpace application. It is also possible to call external programs when needed.

Every executor provides at least following operations:

- **login** - starts session with computational resource using credentials passed by GridSpace user. Currently the credential may be a pair of login and password or a proxy certificate recognized by remote resource
- **execute** - executes passed command with given arguments and script code. It also handles staging in input files and staging out results.
- **logout** - closes session with computational resource and terminates all connections opened by login operation

Each executor is associated with a single File Manager. This file manager is an interface for handling files and directories on remote computational resource. It provides operations for copying, reading, creating and deleting entries using concrete protocols (such as SCP, GridFTP, WebDAV). It is also used for staging in and out. Usually a file manager is created when an exector establishes a session with remote resource (**login** operation).



Executor and FileManager interface

The executor abstraction enables GridSpace to communicate with various types of computational resources with different kinds of protocols. An example is SSH-based implementation that uses SSH protocol for authentication and executing scripts. It can be used to access single sites or nodes. In this case the **login** operation establishes a SSH session with chosen machine and **executing** causes a remote command to be invoked using this connection. It also facilitates SCP protocol client for managing resources on remote machine.

5.6.2 GridSpace Executor for QCG

GridSpace communicates with QCG resources using dedicated Executor implementation. It handles standard executor operations as follows:

- **login** establishes GridFTP session with designated GridFTP server using GSI authentication. Credential is proxy certificate passed by user through GridSpace web interface. The GridFTP session is used by a GridFTP file manager associated with this executor
- **execute** operation submits a job profile generated by GridSpace. This profile contains the command, script code and location of input and output files passed as arguments to this operation.
- **logout** closes established GridFTP session

As mentioned before this executor uses GridFTP for managing files and directories on remote resource. All input files are staged in using this protocol before job is submitted and are staged out right after the job finishes.

5.6.2.1 Running MUSCLE from GridSpace on QCG resources

Mapper tools, namely GridSpace along with Mapper Memory Registry (MaMe) and Multiscale Application Designer (MAD), address Mapper concept to allow for ad-hoc composition of multiscale applications from building blocks of MML entities that are to be registered and made available for application designers. In particular, MML submodules and mappers can be implemented as MUSCLE kernels. MaMe, MAD and GridSpace have to collaborate with each other in order to be able to generate an arbitrary MUSCLE application in a form of GridSpace experiment. Generic mapping of an arbitrary GridSpace experiments to corresponding QCG JobProfiles has also to be ensured in order to enable execution of all existing and potential future MUSCLE applications through QCG.

The problem is to ensure that all jar files being referred to in cxa generated by MAD (lines: m.add_classpath "...", and m.add_libpath "...") are present on the site where MUSCLE kernel is to be executed. MUSCLE kernels (respective to MML submodels or mappers) depend on

several bundles that need to be in place on target site in the location specified in cxa. In order to ensure it, collaboration between MaMe, MAD, EW, QCGBroker and QCGComputing is indispensable.

In MaMe each MUSCLE kernel has assigned bundle names which is a colon-separated list of bundle names, and individual bundle name is qualified using slashes. MAD generates cxa code basing on the information from MAD. Cxa, then, contains the lines as follows:

m.add_classpath
“#{ENV'MUSCLE_KERNEL_REPO'}/mykernel/my.jar:#{ENV'MUSCLE_KERNEL_REPO'}/mykernel/another.jar:#{ENV'MUSCLE_KERNEL_REPO'}/mykernel/classesdir/”

m.add_libpath ”#{ENV'MUSCLE_KERNEL_REPO'}/mykernel/my.so”

Moreover, kernel instance definition in cxa follows the syntax “<kernel_name>_<unique_instance_number>” e.g.

cxa.add_kernel('mykernel_001', '...')

In Experiment Workbench users can pick QCGExecutor to execute cxa snippet. As QCG needs additional information from user on how to distribute kernel instances, user must fill in a form. User specifies the site to be used and for each site a list of kernel instances to be dpeloyed there, number of cores to be allocated and optionally reservation id. Users can but don't have to specify site name and reservation id fields. If site name is not specified it's QCGBroker's role to find suitable sites satisfying number of cores and availability of kernel bundles. In this case QCGBroker uses information from internal registry or external Information System to find suitable sites for given kernels. Kernels are identified by their names, the same that are used in MaMe. After that, QCGBroker dispatches execution of kernels to the QCGComputing installed on found site. On the site QCGComputing executes MUSCLE. Since cxa refers to MUSCLE_KERNEL_REPO environment variable, this has to be set in prior to execution of MUSCLE. This variable keeps a path to site-local repository of kernel bundles e.g. /public/muscle_kernels that is configured in QCGBroker or QCGComputing.

5.6.3 GridSpace Executor for AHE

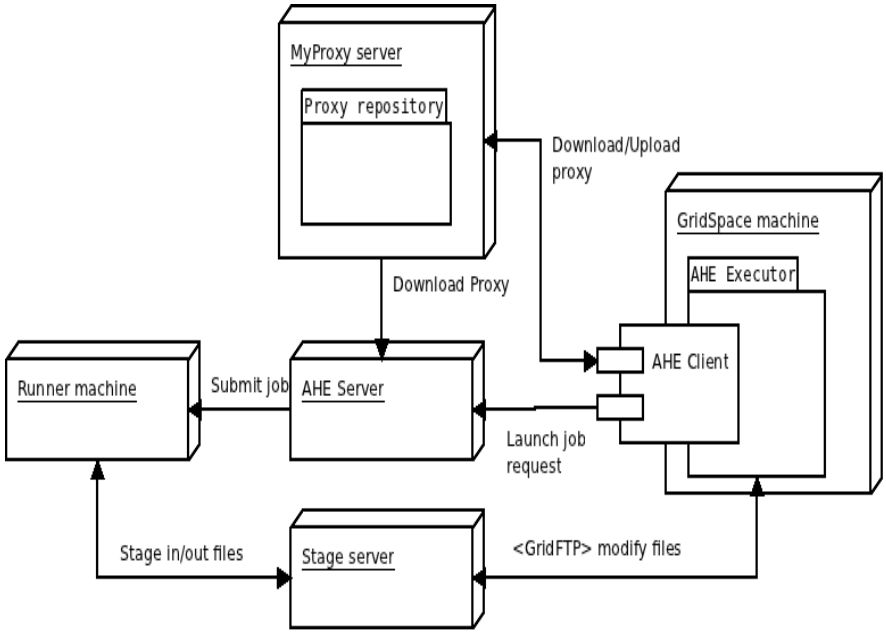
This implementation is currently under development. It uses modified AHE Client written in Java for authentication and executing jobs. The modifications were made so that the client is easily embeddable in other Java applications.

Following list describes planned functioning of operations of this executor. It is unlikely that any of it will change in the future as all of the design has already been discussed with AHE authors.

- **login** - implementation of this operation is almost finished and is in testing phase. Allows two ways of authentication:
    - *proxy certificate* - when provided, executor will send it to AHE MyProxy server through AHE Client and bound to temporary user name and password generated by the executor. This user name and password are later used to authenticate when submitting job to AHE runner machine.
    - *user name and password* - when provided (and no proxy is present) executor attempts use them to authenticate with MyProxy and download valid proxy certificate (that should have been uploaded before using third party client).

In both cases the executor establishes a GridFTP connection with file stage server that the runner machine will use for staging in/out.

- **execute** - not fully implemented. It uses modified AHE Client to create and submit AHE Job Object to AHE runner machine (such as Mavrino). This job objects points to special AHE application called *gslaunch* that is designed to execute scripts on behalf of GridSpace user. When submitted, the AHE Client is set to await mode that periodically polls the job runner for its status. Whet it is finished the operation returns. The AHE Client used by this operation does not stage in or out any inputs or outputs (this is different from behavior of the standalone client). This is because all resources needed for job execution are managed by GridSpace directly on the stage server and therefore are already in place.
- **logout** - connection to the stage server is closed. If temporary password and user name where created by login operation they are cleared.



Above picture shows connection between particular elements in GridSpace- AHE integration. The AHE Executor working on GridSpace machine communicates with MyProxy server through AHE Client and with Stage server using GridFTP client. The runner machine stages in/out input from/to the aforementioned stage server.

Master algorithm is as follows:

- Proper number of nodes is allocated through PBS. This is done as one singe allocation (by using pbsdsh tool)
- The TaskManager is started.
- On each of the assigned nodes a Task process (Slave) is started (via pbsdsh tool) that connects to TaskManager using DRb.
- As asked by a Task, TaskManager sends request to start the plumber
- As asked by a Task, TaskManager sends requests to start appropriate group of kernels
- TaskManager prints the received Task's output to the screen.

Slave algorithm is as follows:

- Task connects to Task Manager using DRb and asks it for a job description
- Task receives a job description (request for staring a plumber or the kernels in a single group)
- Task redirects the output and error streams to the Task Manager

In a case of SSH accessible resources the computational nodes share filesystem with the Experiment Host, so the output files are seen immediately by File Browser which is a standard part of GS Experiment Workbench. The details can be found in (Rycerz-DMC2011).

5.7 Cross-tool integration efforts in MUSCLE

As MUSCLE is meant as a low-level tool, to implement multiscale models in, no changes to MUSCLE have been made to enhance cross-tool integration. However, both QCG-Broker and Gridspace have been adapted for MUSCLE, which is listed in the respective paragraphs.

5.8 Cross-tool integration efforts in AHE

Integration between AHE and other tools in the MAPPER infrastructure happens in two directions: higher level tools are coupled to AHE to act as clients, and AHE is coupled to lower level tools, to facilitate submission. These two integration types are classified as upstream integration and downstream integration respectively, and are discussed in the sections below.

5.8.1 Upstream Integration

Upstream integration has involved coupling AHE with GridSpace, to allow applications hosted in AHE to be called as components of a GridSpace managed workflow. Initially, this was done by preparing shell scripts which automate the launching and monitoring of an AHE hosted application, by calling AHE client commands to prepare and start the application, and then polling the application's state until it is completed. These scripts are then treated as atomic operations by GridSpace, and can be used as the building blocks of workflows.

To coupled AHE more cyclically with GridSpace, we have worked to make it possible to call the Java AHE client API directly from GridSpace. Due to compatibilities between different versions of the same library used by AHE and GridSpace, we had to update the AHE client API to use newer versions of the libraries, which involved some code refactoring. We also updated AHE client to use the Maven library loading system, in order to be further compatible with the way GridSpace worked. We aslo make changes to the way AHE uses proxy certificates to further enhance compatibility between AHE and GridSpace, and developed interface classes which allow the AHE to be controlled by GridSpace.

In addition to updates to the client API, we also developed generic wrapper scripts to allow GridSpace to execute arbitrary applications via AHE. GridSpace needs the ability to execute arbitrary tasks on HPC resources, for example to pre and post process data and run simulations. The generic wrappers allow GridSpace to execute any required tasks, via AHE.

5.8.2 Downstream Integration

The downstream integration efforts have consisted in extending AHE to submit jobs via the QCG BES interface, now deployed on the majority of MAPPER resources. This has entailed creating a new connector to allow AHE to submit jobs to QCG-Computing, and also modifications had to be made to AHE server to enable it to stage files between sites (previously, AHE server relied on the resource manager to perform file transfers).

Additionally, AHE has been extended to allow jobs to be submitted to into reservations created by the QCG Broker. AHE's existing advanced reservation model has been updated, entailing changes to both the client and server, to allow reservations created using QCG to passed through to QCG-Computing when jobs are submitted.

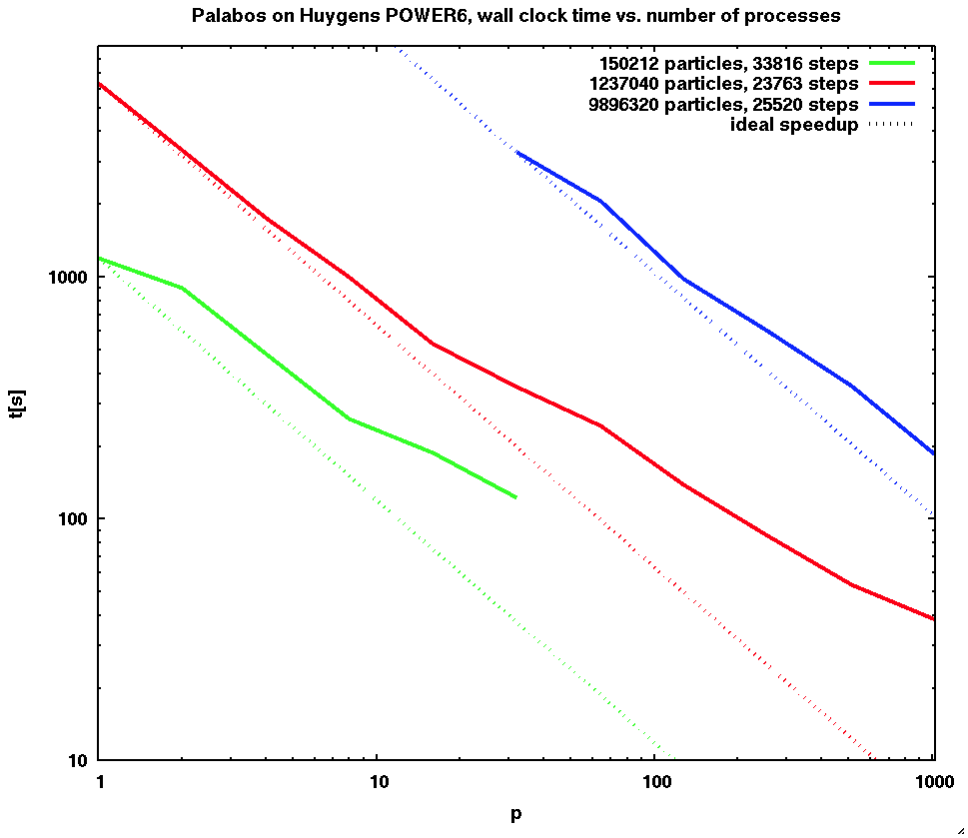
6 Appendix B: Detailed software testing report

6.1 ISR3D

This page contains a range of performance benchmarks for the subcodes used in the In-Stent Restenosis application

6.1.1 Palabos benchmarks

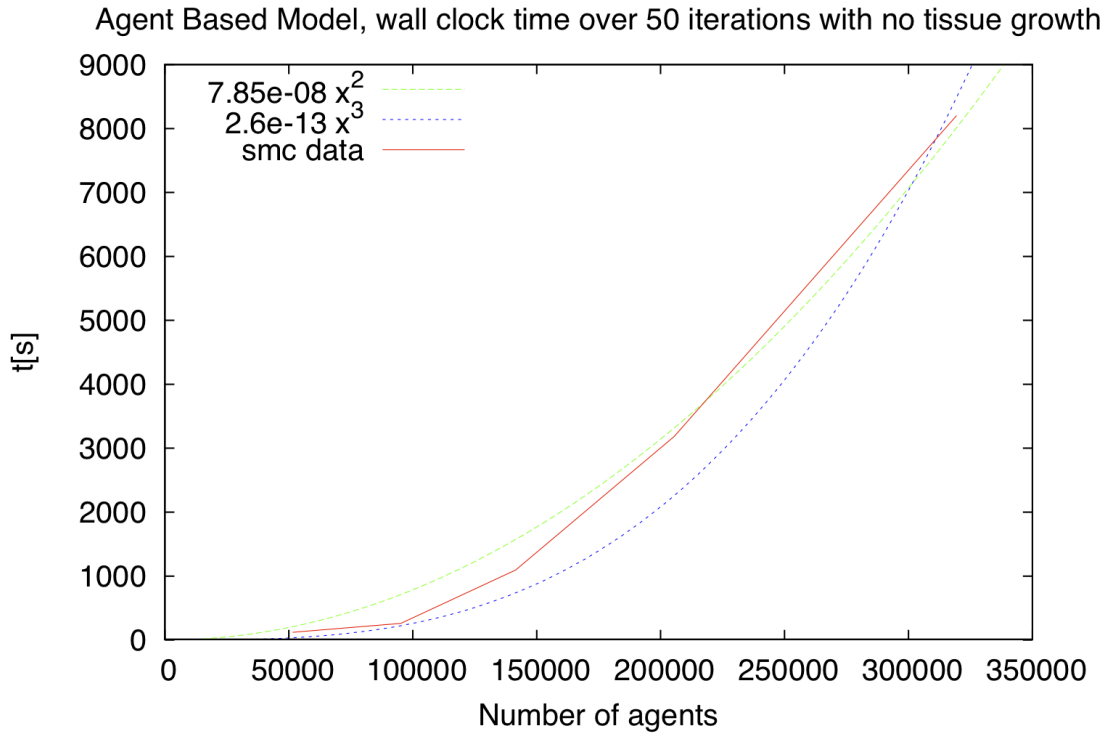
We have benchmarked our Palabos implementation of blood flow dynamics on the Huygens supercomputer at SARA in Amsterdam. This 65TFLOP/s machine is equipped with around 3456 IBM POWER6 processors. We provide the wall-clock time spent to run atomistic simulations until they converged as a function of the number of processes in the figure below. The number of steps is the number of steps it took the code to converge for a given geometry, being the number of particles an indicator of the size of the geometry (length of the artery) simulated. In each In stent restenosis simulation for porcine arteries there are approximately 200 geometry changes, therefore the code needs to converge 200 times.



Scaling was good, specially for a large number of particles.

6.1.2 SMC benchmarks

We have benchmarked our Agent Based Model for Smooth Muscle Cell (SMC) dynamics in a local machine as the code is not yet parallel. The machine is an iMac with intel i5 processors at 3.6 GHz. We observe the wall clock time against the number of agents used. The amount of time it takes the code to complete an iteration is highly dependent on the amount of cells that grow in that iteration, therefore the benchmarks shown below do not include any growth.



We tried to fit the results to a sqared or a cubic scaling with the number of agents. As said, all the simulations for benchamarking of the SMC submodel were carried out without cellular growth in order to minimise the variability between different runs.

6.2 Nanomaterials

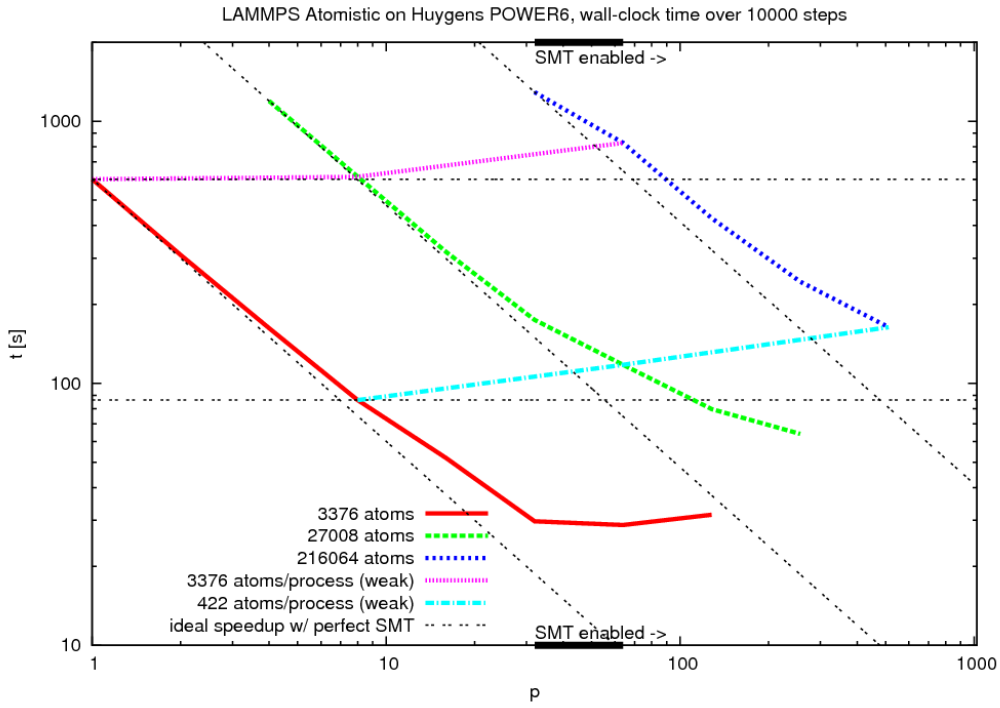
6.2.1 CPMD benchmarks

We have not performed scalability tests of CPMD, as we currently only calculate the potentials of a single clay sheet edge within our multiscale application. However, a report on several scalability tests can be found at: http://www.hpcadvisorycouncil.com/pdf/CPMD_Performance_Profiling.pdf

6.2.2 Atomistic LAMMPS benchmarks

We have benchmarked a range of atomistic simulations of nanocomposites on the Huygens supercomputer at SARA in Amsterdam. This 65TFLOP/s machine is equipped with around 3456 IBM POWER6 processors. We provide the wall-clock time spent to run atomistic simulations for 10000 steps as a function of the number of processes in the figure below.

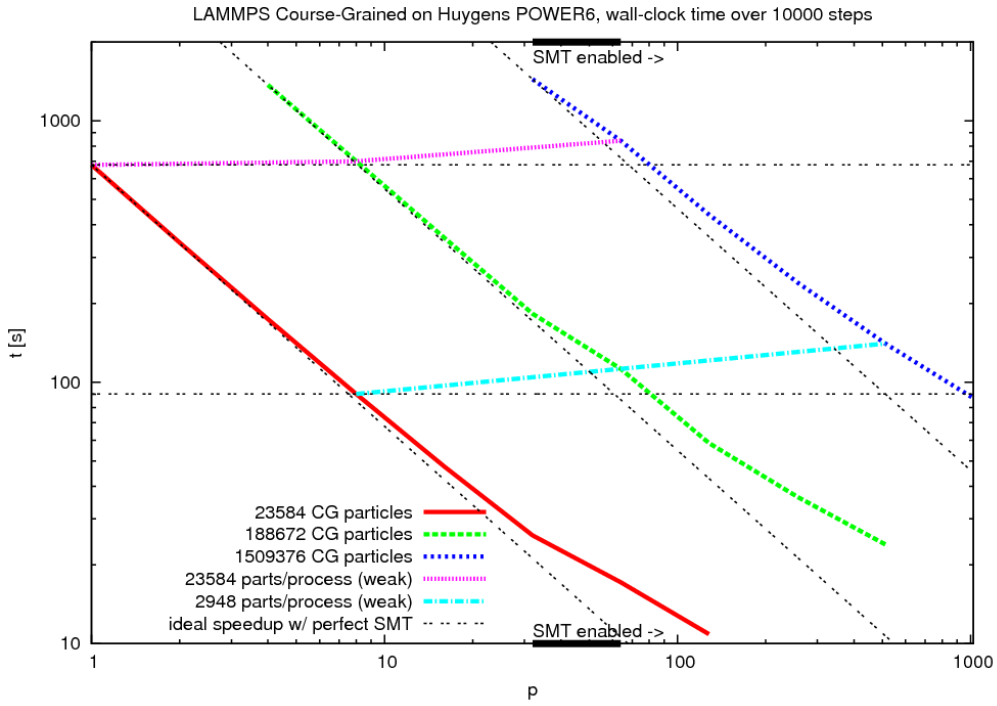
In our application we use SMT to run 2 processes on a single core. Although this somewhat worsens the overall scalability in the plot below, it also allows us to save 50% on our consumption of compute resources. We have enabled SMT in all our tests that use more than 32 cores. The idealized speedup lines do not take the inefficiency introduced by using SMT into account.



6.2.3 Course-grained LAMMPS benchmarks

We have benchmarked a range of course-grained simulations of nanocomposites on the Huygens supercomputer at SARA in Amsterdam. We provide the wall-clock time spent to run course-grained simulations for 10000 steps as a function of the number of processes in the figure below.

In our application we use SMT to run 2 processes on a single core. Although this slightly worsens the overall scalability in the plot below, it also allows us to save 50% on our consumption of compute resources. We have enabled SMT in all our tests that use more than 32 cores.



6.3 QosCosGrid

We decided to measure the performance of the administrative layer component of the QosCosGrid stack: the QCG-Computing service. The benchmarking tests concerned the job submission and job management operations, which are the primary duties of any Basic Execution Service. The proposed two types of the benchmarks aim to measure two important performance metrics: response time and throughput. As nominal values would not provide qualitative answer to the question: "Is the service performance rewarding?" we decided to conduct comparison tests where we compared the performance of the QCG-Computing with similar services: gLite CREAM CE `[footnote:[http://grid.pd.infn.it/cream/]]` and UNICORE UAS `[footnote:[http://unicore.eu/].]` All the tests were performed using a benchmark program written exclusively for the needs of these tests. The program was based on the SAGA C++ API SAGA. Especially the two following SAGA adaptors (i.e. implementations) were exploited:

- glite_cream_job (based on glite-ce-cream-client-api-c) - used to access the gLite CREAM CE service,
- ogf_hpcbp_job (based on gSOAP) - used to access the OGSA BESBES interfaces of UNICORE Atomic Services (UAS) and QCG-Computing service.

The use of the common access layer minimized the risk of obtaining distorted results due to bottleneck in the client layer. Moreover, for the same reason, we decided to use the same target resource for all benchmarks and middlewares.

6.3.1 The Testbed

The testbed was composed of two systems, each of them located in separate networks, connected with Pionier[footnote: [http://www.pionier.net.pl/online/en/]] Wide Area Network.

6.3.1.1 Client Machine

The client machine was a commodity HPC system. The base paramaters of the test system were as follows:

- processors: 2 x 4 cores (Intel(R) Xeon(R) CPU E5345),
- physical memory: 11 GB,
- Operating System: Scientific Linux 5.3,
- RTT from the client machine to the cluster's frontend: about 12 ms.

6.3.1.2 Target Resources Provider

The target site was a one of the Polish NGI PL-Grid cluster: Zeus (88. place on TOP500 list [footnote:www.top500.org/]). This HPC system can be characterized by the following parameters:

- queueing system: Torque 2.4.12 + Maui 3.3,
- about 800 nodes,
- about 3-4k jobs present in the system,
- scheduler poll interval: 3.5 minutes,
- operating system: Scientific Linux,

For the purpose of the tests a subset of 8 nodes (64 cores) where assigned exclusively for the 10 user accounts used for a job submission. The benchmarked services were deployed on separate virtual machines of the following properties:

- Operating System: Scientific Linux 5.5,
- 1 virtual core, 2GB RAM (QCG-Computing and UNICORE)
- 3 virtual cores, 8 GB RAM (gLite CREAM)

6.3.2 Benchmark 1 - Response Times

For the first benchmark we developed a program that spawns N processes (each process can use a different certificate - i.e. act as different user) that invoke the function `sustain_thread`. Next, it waits until all the running processes have ended.

In general, the idea of the program is to keep in a system `jobs_per_thread` jobs for predefined `test_duration` seconds and polling all the time about the job statuses (the delays between successive `query_state` calls drawn from a predefined interval: `SLEEP_COEF`).

The following snippet shows a pseudocode of the function `sustain_thread`:

```
1. start_timer()
2. for i = 1 .. jobs_per_thread
  2a: submit_job(job[i])
3. while (current_time < test_duration) do
  3a: for i = 1 .. jobs_per_thread
  3a1: if (! is_finished(job[i].last_state))
    3a11: sleep((rand() / RAND_MAX) / SLEEP_COEF)
    3a11: query_state(job[i])
  3a2: if (is_finished(job[i].last_state))
    3a21: submit_job(job[i])
4. stop_timer()
```

The function `submit_job(job)`:

```
1. start_timer()
2. job.job = service.create_job()
3. job.job.run()
4. stop_timer()
5. query_state(job)
```

The function `query_state(job)`:

```
1. start_timer()
2. job.last_state = job.job.get_state()
3. stop_timer()
```

At the end of tests, the average, minimal and maximal times of submitting a job (`submit_job`) and querying about a job state (`query_state`) are printed. Additionally, the program displays the number of all submitted jobs, the number of successfully finished jobs

(*Done*) and the number of the jobs finished with the other status (*Canceled*, *Failed*). In the last case, the number of failures, i.e. exceptions thrown by the SAGA adaptors, is shown.

6.3.2.1 Test Runs

Every test was characterized by: maximal number of jobs per user, number of users (concurrent processes), total number of jobs, test duration and maximal sleep time between every successive `query_state` call. We conducted four test sets, for every of the three tested middlewares, the paramaters of the tests are listed below:

- 50 jobs x 10 users = 500 jobs, 30 minutes, SLEEP_COEF = 10 seconds,
- 100 jobs x 10 users = 1000 jobs, 30 minutes, SLEEP_COEF = 10 seconds,
- 200 jobs x 10 users = 2000 jobs, 30 minutes, SLEEP_COEF = 10 seconds,
- 400 jobs x 10 users = 4000 jobs, 30 minutes, SLEEP_COEF = 10 seconds.

Results

- The average submit time of a single job

Test	QCG 2.0	UNICORE UAS	gLite CREAM
50	1.43	2.41	8.47
50x10	1.43	2.41	8.47
100x10	1.49	1.24 a	8.45
200x10	1.99	2.20	8.50
400x10	1.96	- b	8.24

- The average time of a query about a job status.

Test	QCG 2.0	UNICORE	gLite
50x10	0.38	2.73	0.20
100x10	0.35	1.61	0.36
200x10	0.63	3.73	0.24
400x10	0.47	- b	0.21

6.3.3 Benchmark 2 - Throughput

The test is based on the methodology described in the paper BENCH. Similar to the approach described in the paper we aimed to measure the performance from the user perspective. The test procedure consisted of two phases:

- submitting sequentially, one after another, N jobs into the target system,
- waiting until all jobs have ended.

The test job was a No OPeration (NOP) task, that finishes immediately after starting. We measured the time between the submission of the first job and the finish of the last job. Our improvements in the test methodology, over the aforementioned publication, were:

- submitting the jobs using *k* processes/users,
- using one client API (SAGA) instead of the command-line clients,
- single, real production, testbed environment.

6.3.3.1 Test Runs and Results

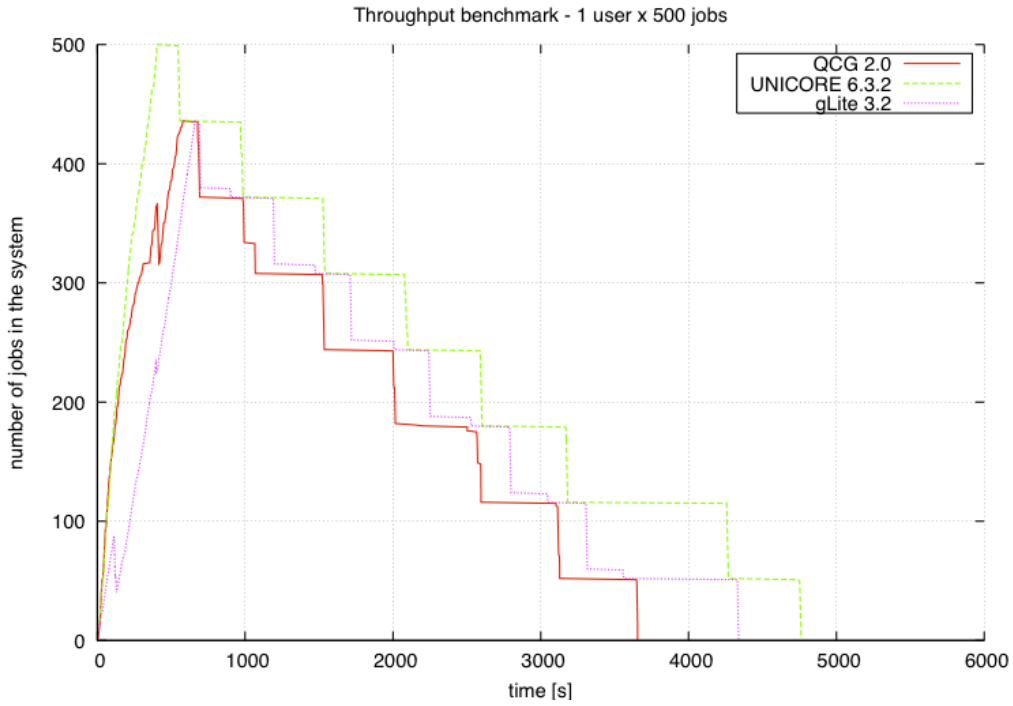
The test sets were parametrized by the following parameters:

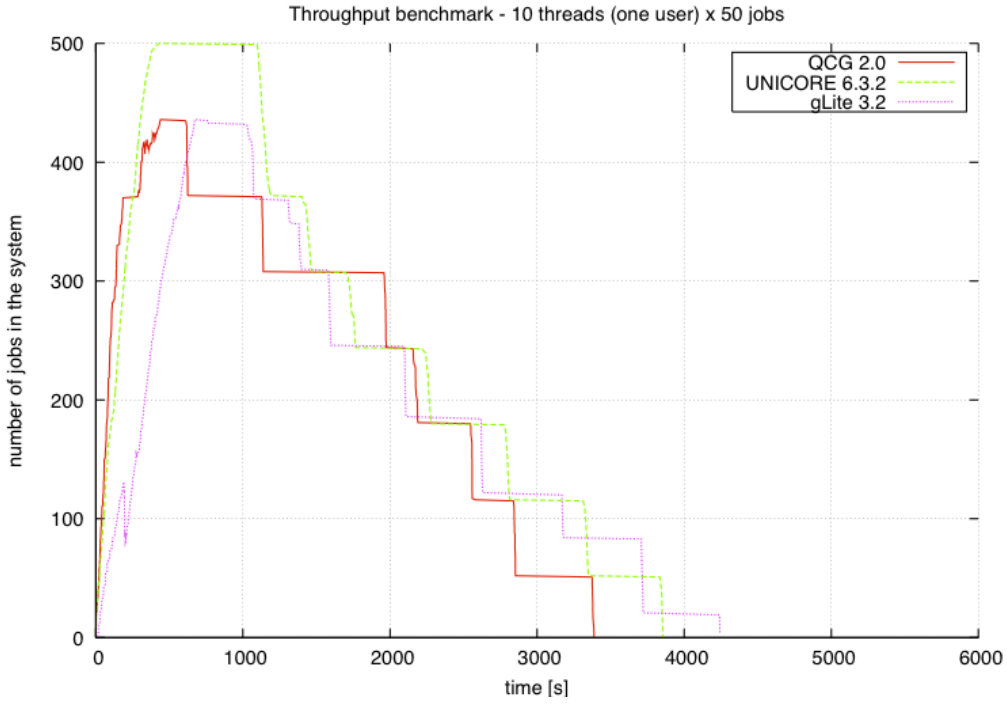
- number of concurrent threads (*k*),
- whether all threads used single client certificate or not,
- total number of jobs (*N*).

Altogether we ran 4 test-sets characterized by the following parameters:

- 1 user, 1 thread, 500 jobs,
- 1 user, 10 thread, 500 jobs (50x10),
- 10 users, 10 thread, 500 jobs (50x10),
- 10 users, 10 thread, 1000 jobs (10x100).

The results are presented in the figures below:




Throughput benchmark - 10 threads (one user) x 50 jobs
QCG 2.0
UNICORE 6.3.2
gLite 3.2
number of jobs in the system
time [s]
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400
500
0
1000
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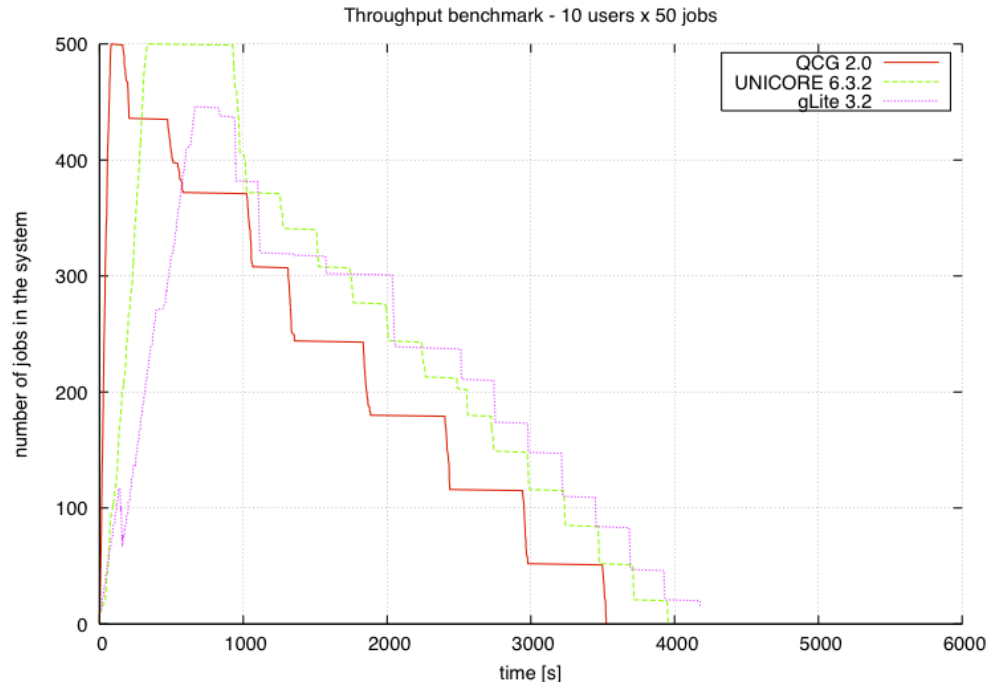
3000
4000
5000
6000


Throughput benchmark - 10 users x 50 jobs
QCG 2.0
UNICORE 6.3.2
gLite 3.2
number of jobs in the system
time [s]
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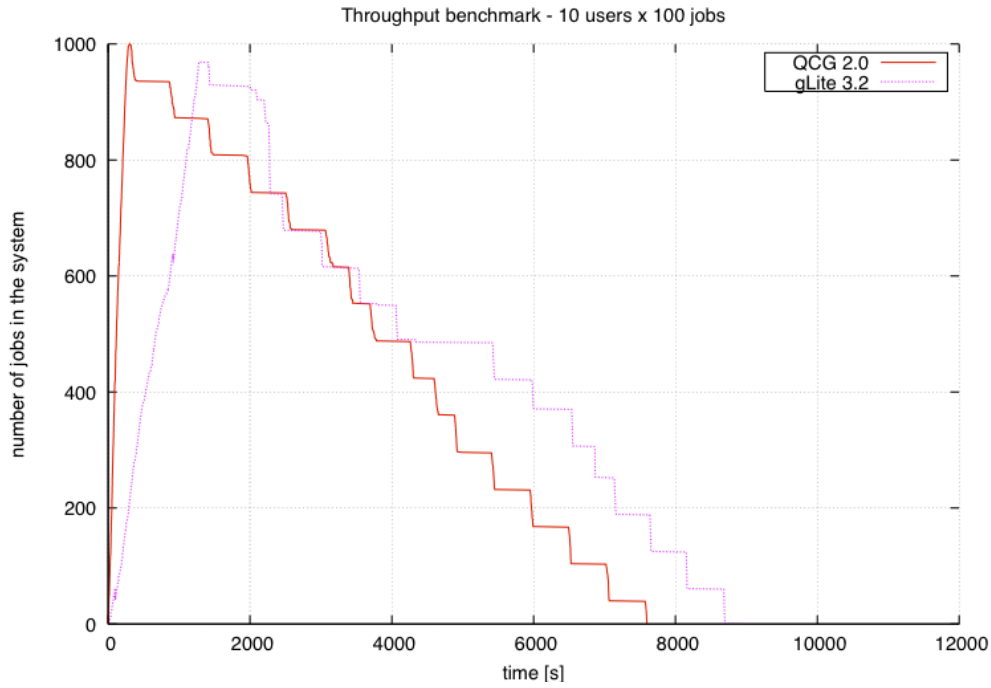


Unfortunately in the second benmark the bottle-neck was the throughput of the Maui scheduler and size of the dedicated testbed partition (8 machines), which imposed that only 64 jobs could be scheduled per one scheduling cycle (at least 3.5 minutes).

6.4 GridSpace

6.4.1 Tools Usability Tests

During first MAPPER seasonal school, we have performed usability tests of MaMe, MAD and GridSpace Experiment Workbench tools based on: John Brooke Usability evaluation in industry, SUS—a quick and dirty usability scale (CRC Press, Boca Raton, FL), pp 189–194 (1996) . After making assignments (available on http://www.mapper-project.eu/web/guest/mad-mame-ew), the school participants were asked questions about usability of the system they used. The obtained average SUS score for the tools was 68 points (for 100 possible; standard deviation was 18) . The average was calculated from answers from 10 participants.

As the tools are still under the development we have also collected specific remarks that could potentially help to improve their usability. The request from most of the participants was to improve interface for parameter management of application submodules. Currently, we are working the improvements. We also plan to perform similar tests during the second MAPPER seasonal school planned in M30 of the project.

6.4.2 GridSpace Continuous integration and testing

The Grid Space project uses continuous integration for building and testing applications. The Continuum integration server builds whole application every 4 hours. Each build consists of compiling, running unit and integration tests (see in following sections) and assembling an application to a package (jar or war). The main goal of this process is to ensure that the developers are constantly notified about errors in code correctness or functionality so that they can react appropriately The Continuum server is also responsible for deploying latest version of Experiment Workbench tool to a development web application server. Thanks to that the latest development version of the application is automatically available for manual testing or using.

During the development of GridSpace EW we have written integration and unit tests that check the correctness and usability of this tool. Both kinds of tests were written in Java using the Junit library. More detailed description follows.

6.4.2.1 Unit tests

These tests concern single functionality and behavior of piece of Java code (like method). We ensure maximum isolation of particular tests from other parts of the system using *mock* code created with Mockito library. Additionally, we sometimes use unit tests for *documenting* a bug found in the code. Such test reproduces programatically the conditions the problem occurred in and reduces the probability that previously fixed defect will reappear unnoticed.

Because these tests are usually simple and fast to execute they are used to pinpoint the erroneous code and quickly check functionality being developed.

6.4.2.2 Integration tests

Integration tests first set up a testing environment consisting of a few components and optionally a connection to external system and invoke some operations on subjects of the test. The examples are QCG executor component tests which connect to external QCG server and login to dedicated testing account on the QCG broker. Then the test code invokes an *execute* operation and checks whether the operation was successful and the expected output appeared. This is performed using different configurations of the execution process and different experiment snippets. Similar tests for integration with AHE are currently being written together with the main code.

The integration tests facilitate keeping whole application working and detecting errors caused by changes in communication interfaces with external systems. Much like the unit tests they also ensure that during the development old functionality is maintained. Howerev, they they are usually longer and more complex.

6.4.2.3 Code coverage

To present the quality of our tests we use metrics called *code coverage* that gives a degree to which code have been tested. In our case it is evaluated using two criteria:

- number of lines of code invoked during tests to total number of lines of code (*line coverage*)
- number of code branches that get invoked during tests to total number of code branches (*branch coverage*)

The following table presents code coverage for each GridSpace Experiment component. All values are expressed as percentage and where gathered using the Cobertura tool.

Component Name	Component description	Line coverage	Branch coverage	#Classes
EW*	Experiment workench web application	8	4	139
core	Core utilities and interfaces	45	32	45
executors	definition of interfaces for integration with external computational resources	0	0	30
provenance	gathering and storing provenance data	49	32	30
experiment	basic interfaces and classes for handling experiment definition	47	13	19
ssh-executor	executing experiments using ordinary SSH connection and authentication	47	31	22

*-excluding GWT's *client* packages

When interpreting these results one should keep in mind that the EW component is mainly a web-based application that provides GUI and uses other components for executing an experiment. Unit and integration testing is not suitable for such applications and therefore the code coverage is relatively small in this case.

6.4.2.4 Performance, reliability and conformance tests of Experiment Workbench

As GridSpace2 Experiment Workbench is still in development phase the ultimate performance, reliability and conformance tests are expected in the future. However, the architecture and design patterns being applied in the software already follow the good practices in testing which will allow for carrying out such tests during the software evaluation and optimization phase.

Experiment Workbench being a web application inteded to enable pervasive access for the users using web browsers needs to be examinated in terms of browser compatibility including all major web browsers according to e.g StatCounter wordwide analysis published annually. As for 2012 their analysis show that MicroSoft Internet Exporer (29.05%), Google Chrome (23.22%), Mozilla Firefox (21.76%), Safari (13.49%), Opera (5.2%) are the key vendors taking almost 92.72% of the market. Experiment Workbnech must be supported by the most up-to-date version of these browsers and their previous versiosn in order to ensure both long-term support from these browsers and availability for expected treshod of 75% of web browser users.

To meet this indicator Experiment Workbench is taking advatage of web frameworks (mostly Google Web Toolkit) which by design addresses the cross-browser compatibility concern. Moreover, by applying Model-View-Presenter design pattern the browser-specific layer is made as thin as possible, thus greater part of the code is web browser-agnostic.

The performance aspect can't be underesimated as it determines scalability of the solution in terms of resources and costs to be born in order to ensure desired system throughput. The metrics used to measure the throughput will be:

- A number of benchmark experiments being excuted in parallel through the same instance of Experiment Workbench with a given amount of hardware resources. Computational demands of benchmark experiments are irrevelant in this case as they introduce load on execution backend (grid sites) while capability being examinated is the throughput of the Experiment Workbench. This will give estimation of hardware resources usage by a single benchmark experiment run.
- A number of open user sessions to the same instance of Experiment Workbench with a given amount of hardware resources. This will help investigate the minimal resources footprint that is generated by a single user session.

Performance tests will be easy to develop owing to the model-view-presenter design pattern being applied in Experiment Workbench. In conjunction with gwt-syncproxy library they provide a way for automatic testing of functionallity without a must of running brower-side user interface.

In addition to that, the reliability tests will be carried out by monitoring the instances of Experiment Workbench under a real or artificially generated load. This will help identify longundesired long-term effects e.g. resource leaks.

6.4.3 Mapper Memory Registry (MaMe)

The Mapper Memory Registry is a standalone server, which uses its persistence layer in order to provide storage and publishing capabilities for a range of MAPPER use cases (module registry, XMML repository). For more details on its internal structure, please consult e.g., Section 8.2.2.3 in D8.1 deliverable.

MaMe utilizes the model-view-controller methodology for its internal architecture and, as such, need these three elements tested. We have approached to the problem threefold: by designing and applying a set of unit testing for model and controller layers, by measuring the performance of REST publishing element and by testing compatibility of the view layer with the newest web browsers.

Unit testing. The domain model of MaMe (comprising several different entities which are subject of publishing and sharing inside the registry), its structure, consistency and validity, is being continuously tested by a set of unit tests. Also, the controller layer, which, apart from the basic CRUD set of operations, provides more complex capabilities, is being tested with a separate set of unit tests. Altogether the validity of these two layers are tested by a set of 87 assertions (as of 12.03.2012) and that set grows with any new functionality being added to MaMe (test-driven development).

MaMe is a standalone server and, as such, does not require any integration testing (or, for that matter, continuous integration setup). It is, however, advisable, that other tools which use MaMe through its REST API, deploy such techniques, for integration testing.

Performance testing. As MaMe provides a set of REST APIs, for other elements of Mapper Toolbox, it is useful to measure the performance of these endpoints. Out from the complete set of REST operations, we have chosen three representatives, to measure how quickly they are capable of returning a valid response. All tests are taken on the production deployment of MaMe from a local computer (this resembles quite accurately the usual user environment, where tools like MASK or MAD contact MaMe for some metadata).

For the first test, we have chosen the `[models_list]` operation, as the most demanding - it takes the whole list of Submodules, Mappers and Filters inside the registry, builds a single JSON document (around 150 kB) and returns it to the caller. We performed several hundreds calls and the entire operation takes about **0.83 seconds** client-side. This includes connection establishment and the TCP handshake. On the server-side, the same operation takes **0.58 seconds** (the rest **0.25 seconds** is taken by request preparation, communication and demarshalling of the response). However, when the HTTP connection is being reused from call to call (the usual mode of operation for MaMe clients like MASK and MAD), the performance rises to **0.64 seconds** on the client-side (total wall-clock time). Since this is a

kind of holistic operation, it is designed to be called quite infrequently (probably once for every user login to MAD) - and this allows us to decide such a delay is acceptable.

In order to measure less demanding, faster operation, we have performed similar tests for the `[experiments_lis]` API endpoint. It returns a smaller JSON document (a little more than a kilobyte) and it requires MaMe to perform much smaller database lookup. For the entire operation, the wall-clock time on the client side is **0.046 seconds** (out of which **0.013 seconds** are spent in the server). In the connection reuse mode, the entire operation takes **0.021 seconds**. Clearly, here much higher impact is introduced with the connection and handshake procedures.

Finaly, to also measure update (write) operations performance, we used the `[add_base/Filter]` operation to add many new Filters to the registry. In contrary to two above methods, this requires basic authentication and relies on the POST HTTP method (not GET). However, due to very small amount of information being exchanged between the client and MaMe, the entire procedure takes only **0.037 seconds** on average (including the authentication). This figure we also find acceptable.

Browser conformance testing was performed manually, by using MaMe's web UI from various Web browsers. At the moment of writing this deliverable, MaMe UI works properly with Internet Explorer (ver. 9.0 running on Windows 7), Chrome (ver. 17.0 on both Linux and Windows 7), Opera (ver. 11.50 on Linux and ver. 11.61 on Windows 7) and Firefox (ver. 10.0 on Linux).

6.4.4 Multiscale Application Developer (MAD)

MAD is a web application providing convenient and user-friendly set of tools allowing users to compose Mapper applications and export them to executable experiments inside GridSpace Experiment Engine. As a source of information MAD uses the MaMe registry by means of JSON-enabled set of REST APIs. The modules obtained from the registry are combined by users into applications by applying simple drag-and-drop routines inside a web browser. For this to be possible MAD utilizes a few libraries namely Google Web Toolkit as the integration platform, lib-gwt-svg for SVG graphics support and gwt-dnd for handling drag-and-drop. Combination of these requires additional effort to support available web browsers. Currently, as MAD is still being developed, support for latest Firefox and Google Chrome browsers for both Window and Linux platforms is ensured. In future, tweaks to support other major browsers (e.g. Internet Explorer, Opera) will be applied.

MAD relies on external components within the Mapper infrastructure which are MaMe - the model registry and Experiment Workbench - the execution engine. The communication

between the components is implemented by using well-known standards to minimize errors and ensure stability. As the MaMe registry uses JSON notation to share its contents Jackson processor (http://jackson.codehaus.org) and Jersey library (http://jersey.java.net/) were used to parse and produce responses and requests to the registry. The Experiment Workbench on the other hand prefers the XML notation to communicate with external components. In this case one of the JAXB implementations (provided by Sun Java Runtime) was used to ensure stable communication. Use of the mentioned libraries makes the integration stable and requires minimal set of integration tests on the MAD side.

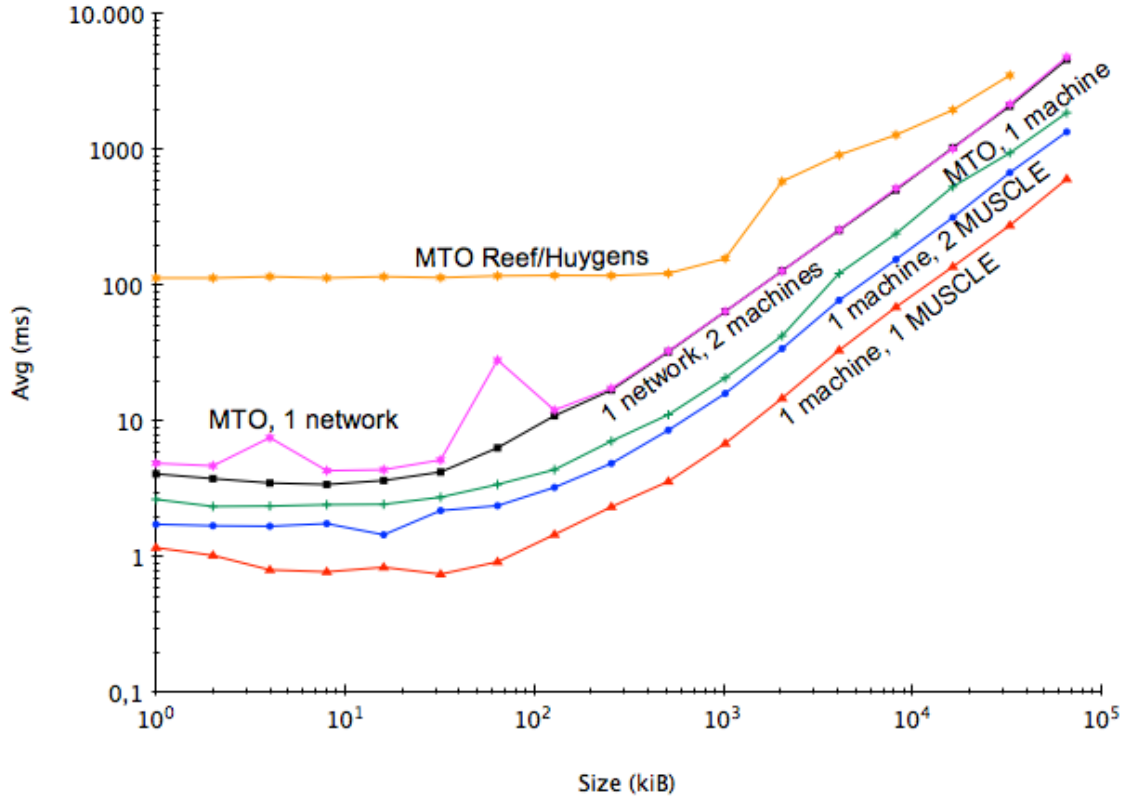
Testing of such highly interactive user interface is difficult to be automated. Existing web testing frameworks (e.g. Selenium) do not support recording of drag-and-drop actions. That is why the structure of the MAD project follows the MVP principles (http://code.google.com/webtoolkit/articles/mvp-architecture.html) which let unit-test user interfaces all the way up to the views. Additionally, the core of the application is abstracted into a set on controllers and presenters independent of the view engine implementation (currently GWT with supporting libraries).

6.5 MUSCLE

MUSCLE has been tested on an single iMac with an Intel i3 3.2 GHz processor running Mac OS X 10.7.3 to measure communication library overheads. It is connected to a dual core Intel 2160 1.8 GHz processor running Ubuntu Server on the same network to measure the influence of using network. In another test, we use MTO between Reef (a PL-Grid resource in Poznan, Poland; a 16-core Intel Xeon E5530 2.4 GHz node) and Huygens (a PRACE Tier-1 resource in Amsterdam, The Netherlands; a 64-core IBM Power6 4.7 GHz node).

6.5.1 Results

The following measurements have been performed so far, by sending messages of different sides from one submodel to another and back, with details in the paragraphs and tables below. Note that the average time is in fact the round-trip time (RTT), of one message being sent to the other submodel and that message repeated to the first. By dividing by two, the time for sending a single message is approximated.



MUSCLE run in a single instance has extremely high communication speeds and low latency, with two MUSCLE instances it is still acceptable, with a latency of less than 2 milliseconds RTT and a bandwidth of 100 MB/sec. On a single network latency is slightly increased at 4 ms RTT and a bandwidth of just 30 MB/sec. The latency comparable but a bit more unpredictable while using MTO, but stays under 8 ms RTT; the bandwidth stays the same. Using MTO on a single machine, both latency and bandwidth seem to suffer slightly. Over a link between Reef (in Poznan, Poland) and Huygens (in Amsterdam, the Netherlands) the latency is higher here, and more than the distance should account for, at around 115 ms RTT. This compares to a ping time of 38 ms, or, three messages back and forth for a single message. The bandwidth fluctuates between 7 and 13 MB/sec. Comparing with the other results, it would seem that this is a problem with the connection rather than due to performance of MUSCLE.

Overall, MUSCLE does not seem to introduce much overhead. Largest factors are whether it is using sockets or within-process communication, and the high latency effect between distant super-computers.

Below are the precise measurement tables.

6.5.2 MUSCLE on a single machine, with a single instance

Each value is calculated for RTT. Sending 10000 messages in total. For each data size, 30 tests are performed, each sending 10 messages.

Size (kiB)	Total (ms)	Avg (ms)	StdDev (ms)	StdDev (%)	Speed (MB/s)
0	404	1.349	0.307	22.726	NaN
1	351	1.172	0.227	19.367	1.747
2	308	1.029	0.284	27.628	3.981
4	241	0.805	0.124	15.473	10.181
8	233	0.777	0.122	15.663	21.089
16	252	0.843	0.184	21.814	38.884
32	224	0.749	0.056	7.499	87.457
64	276	0.921	0.127	13.747	142.280
128	439	1.464	0.191	13.079	179.056
256	702	2.343	0.828	35.351	223.794
512	1080	3.603	0.130	3.596	291.020
1024	2059	6.864	0.191	2.785	305.538
2048	4429	14.766	1.704	11.540	284.050
4096	9993	33.313	3.447	10.346	251.815
8192	20816	69.387	3.837	5.530	241.793
16384	41262	137.541	7.623	5.542	243.959
32768	83177	277.259	4.923	1.776	242.044
65536	182713	609.045	24.691	4.054	220.374

6.5.3 MUSCLE on a single machine, with two instances

In this case, communication is performed over local sockets. Values are NOT divided by 2. Each value is calculated for RTT. Sending 10000 messages in total. For each data size, 30 tests are performed, each sending 10 messages.

Size (kiB)	Total (ms)	Avg (ms)	StdDev (ms)	StdDev (%)	Speed (MB/s)
0	557	1.857	0.250	13.466	NaN
1	521	1.739	0.357	20.511	1.178
2	509	1.699	0.309	18.197	2.412
4	505	1.685	0.653	38.739	4.863
8	528	1.760	1.697	96.429	9.307
16	436	1.457	0.348	23.916	22.497
32	659	2.197	1.936	88.139	29.831
64	715	2.385	0.420	17.622	54.965
128	976	3.253	0.780	23.971	80.575
256	1465	4.887	0.167	3.423	107.291
512	2576	8.588	0.143	1.665	122.097
1024	4806	16.020	0.508	3.170	130.905
2048	10292	34.308	1.899	5.536	122.255
4096	23343	77.812	3.326	4.275	107.807
8192	46679	155.598	3.243	2.084	107.824
16384	95138	317.129	6.000	1.892	105.807
32768	203558	678.529	137.618	20.282	98.903

65536	406353	1354.511	65.008	4.799	99.089

6.5.4 MUSCLE on two machines on the university network

Values are NOT divided by 2. Each value is calculated for RTT. Sending 10000 messages in total. For each data size, 30 tests are performed, each sending 10 messages.

Size (kiB)	Total (ms)	Avg (ms)	StdDev(ms)	StdDev(%)	Speed (MB/s)
0	1227	4.090	0.351	8.593	NaN
1	1227	4.091	0.600	14.673	0.501
2	1132	3.776	0.345	9.127	1.085
4	1051	3.506	0.344	9.815	2.337
8	1025	3.418	0.400	11.716	4.794
16	1097	3.658	0.477	13.035	8.958
32	1267	4.225	0.393	9.301	15.513
64	1909	6.365	1.469	23.087	20.594
128	3291	10.973	2.763	25.176	23.890
256	5093	16.979	2.641	15.556	30.879
512	9724	32.414	3.970	12.248	32.350
1024	19290	64.300	5.404	8.405	32.615
2048	38463	128.213	6.586	5.137	32.714
4096	76489	254.964	19.046	7.470	32.901
8192	151772	505.909	18.913	3.738	33.163
16384	310636	1035.455	34.738	3.355	32.405
32768	628682	2095.609	51.171	2.442	32.024
65536	1387174	4623.915	215.892	4.669	29.027

6.5.5 MUSCLE between Huygens and Reef, using the MTO

Size (kiB)	Total (ms)	Avg (ms)	StdDev(ms)	StdDev(%)	Speed (MB/s)
0	57438	191.461	1.734	0.905	NaN
1	34064	113.549	0.254	0.224	0.018
2	34061	113.537	0.352	0.310	0.036
4	34883	116.280	3.303	2.841	0.070
8	34093	113.644	1.328	1.168	0.144
16	34859	116.197	3.391	2.919	0.282
32	34286	114.290	1.460	1.278	0.573
64	35317	117.726	10.996	9.341	1.113
128	35618	118.728	3.656	3.080	2.208
256	35479	118.264	3.767	3.185	4.433
512	36811	122.705	4.570	3.725	8.546
1024	47435	158.118	72.290	45.719	13.263

2048	175250	584.170	278.434	47.663	7.180
4096	274489	914.966	55.014	6.013	9.168
8192	385815	1286.052	141.569	11.008	13.046
16384	589310	1964.367	235.537	11.990	17.082
32768	1060300	3534.334	316.179	8.946	18.988

6.5.6 MUSCLE between two computers on the local network, using MTO

Size (kiB)	Total (ms)	Avg (ms)	StdDev(ms)	StdDev(%)	Speed (MB/s)
0	12001	40.004	0.238	0.596	NaN
1	1469	4.897	0.257	5.254	0.418
2	1407	4.691	0.376	8.012	0.873
4	2271	7.571	17.180	226.906	1.082
8	1296	4.323	0.750	17.353	3.790
16	1317	4.392	0.254	5.783	7.461
32	1555	5.185	0.458	8.829	12.639
64	8460	28.200	4.517	16.018	4.648
128	3618	12.063	3.217	26.671	21.731
256	5245	17.486	2.365	13.522	29.983
512	9866	32.887	2.656	8.076	31.884
1024	19356	64.520	3.879	6.011	32.504
2048	38328	127.762	4.694	3.674	32.829
4096	77218	257.395	11.366	4.416	32.590
8192	155888	519.628	29.123	5.605	32.287
16384	305093	1016.978	16.594	1.632	32.994
32768	649366	2164.555	49.819	2.302	31.004
65536	1445309	4817.698	80.363	1.668	27.859

6.5.7 Two MUSCLE instances on the same machine, using MTO

Size (kiB)	Total (ms)	Avg (ms)	StdDev(ms)	StdDev(%)	Speed (MB/s)
1	797	2.657	0.450	16.941	0.771
2	706	2.354	0.194	8.234	1.740
4	711	2.371	0.320	13.509	3.455
8	728	2.427	0.873	35.971	6.750
16	732	2.442	0.896	36.684	13.418
32	826	2.756	0.346	12.565	23.777
64	1025	3.420	0.853	24.938	38.328
128	1318	4.396	0.290	6.595	59.638
256	2141	7.138	1.531	21.453	73.454
512	3350	11.167	0.414	3.705	93.901
1024	6251	20.838	0.493	2.366	100.641

2048	12789	42.632	1.065	2.497	98.384
4096	36765	122.551	92.713	75.653	68.450
8192	72287	240.958	85.006	35.278	69.627
16384	160505	535.020	219.298	40.989	62.716
32768	283970	946.567	412.473	43.576	70.897
65536	562114	1873.716	569.141	30.375	71.632

6.6 Application Hosting Environment

AHE is designed to simplify user experience, and as such benchmarking of the tool has involved conducting usability studies to compare AHE to other similar tools.

6.6.1 Usability Study Methodology

Our usability study comprised two sections. Globus and UNICORE are the de facto standard middleware tools used to access contemporary production grids to which we have access. By default, Globus is accessed via command line tools to transfer files and submit and monitor jobs. UNICORE has both command line and graphical clients to launch and monitor applications, as does AHE. The first part of our study compared the usability of the Globus command line clients with the usability of the AHE command line client, and the usability of the UNICORE Grid Programming Environment (GPE) graphical client (which we ourselves found easier to use than the full UNICORE Rich Client) with the usability of the AHE graphical client. The version of Globus used was 4.0.5, submitting to pre-WS GRAM; version 6.3.1 of UNICORE was used, with version 6 of the GPE client. AHE version 2.0 was used for the AHE based tests, with a prerelease version of AHE+ACD used for the security tests.

The remaining part of our usability study set out to evaluate our second hypothesis. We compared a scenario where a user was given an X.509 certificate and had to configure it for use with AHE to a scenario where a user invoked ACD to authenticate to AHE. Both sections of the study can be considered as representing `best case scenarios'. Firstly, all tools were installed and preconfigured for the user. An actual user of TeraGrid or DEISA would most likely have to install and configure the tools herself. In the security section of the study, the user was given an X.509 certificate to employ with AHE. In reality, a user would have to go through the process of obtaining a certificate from her local Certificate Authority, a time consuming task that can take between two days and two weeks.

In passing we note that while other middleware tools, and other interfaces to Globus and UNICORE, certainly do exist, these interfaces are often community specific and not available to all users. Our tests evaluate the default minimum middleware solutions available to TeraGrid and DEISA users.

6.6.2 Participants

Some usability experts maintain that five is a suitable number of subjects with which to conduct a usability study, since this number of people will typically find 80\% of the problems in any given interface. However, our study does not seek bugs in a single interface: it asks participants to compare the features of several middleware tools to find which is most usable. To do this we need a sufficient number of participants to be sure that our results are statistically significant. To determine the minimum number of participants required, we conducted a power analysis, calculating the probability that a statistical test will reject the null hypothesis or alternatively detect an effect. In order to determine the statistical significance of our results, we used a one-tailed paired t-test. For a reasonable statistical power of 0.8 (i.e. the probability that the test will find a statistically significant difference between the tools), we therefore determined we would need a minimum of 27 participants, plus a few more to allow for those who might drop out for various reasons.

We recruited a cohort of 39 participants consisting of UCL undergraduate and postgraduate students, each of whom received a £10 Amazon Voucher for taking part in the study. These participants came from a wide range of backgrounds in the humanities, sciences and engineering, but none had any previous experience in the use of computational grids. This cohort is therefore analogous to a group of new users of computational grids (e.g. a first year PhD student) in terms of educational background and experience.

6.6.3 Tasks

As discussed, our usability study was split into two sections. In the first section participants were asked to compare Globus, UNICORE and AHE by performing three separate tasks:

- Launch an application on a grid resource using the middleware tool being tested. The application in question (pre-installed on the grid resource) sorted a list of words into alphabetical order. The user had to upload the input data from their local machine and then submit the application to the machine.
- Monitor the application launched in step 1 until complete.
- Download the output of the application back to the local machine once it has completed.

The second section compared the use of X.509 certificates to ACD authentication. In this section, users were asked to perform the following two tasks:

- Configure the AHE client with to use an X.509 certificate, and then submit a job using the graphical client.

- Authenticate to AHE using an ACD username and password, and then submit a job using the graphical client.

In order to avoid the typical queue waiting problem when using HPC resources, all of the tests ran the application on the same server, based locally in the Centre for Computational Science at University College London, which was used solely for the purpose of running the usability test application.

6.6.4 Data Collection

Prior to beginning the tasks outlined above, each participant was asked a number of question related to their academic background, general IT experience and previous experience of using grid middleware tools. After each task, we asked the participants to rate the difficulty of the task and their satisfaction with their performance of the task, using a Likert scale (i.e. five options from strongly agree to strongly disagree). In addition, we timed how long it took the user to complete each task. After using each tool, we asked the participant to evaluate it using the System Usability Scale (SUS), via ten questions about his impression of the tool giving a standard measure of usability scored out of 100, which is suitable for making comparisons between tools. After completing the two sections of the study, each participant was able to give freeform comments on impressions of the tools used, if desired. While performing each task, an observer watched each participant and recorded whether or not the task was completed successfully.

6.6.5 Delivery

To ease the process of data collection and tabulation (and the timings of tasks), we developed a simple web platform from which to deliver the usability study. The study was conducted in the Centre for Computational Science at University College London. Each participant in the study was assigned an ID number, which they used to log on to the delivery platform. All of the various usability metrics were then recorded against this ID in a database. Before starting the study, the delivery platform displayed a page explaining to the user the purpose of the study. The observer also explained to the participant that he was not able to provide any assistance or answer questions relating to the tasks being performed.

The delivery platform provided web forms on which participants could record the answers to the questions outlined in the previous section. The delivery platform also described the operations that the user had to carry out. Prior to performing the task, the user had to click a Start button, which set a timer running for the task, and a Stop button when it was completed. When performing a task, the user was given a documentation snapshot, taken from the tool's documentation, that instructed them how to perform the task (included as electronic

supplementary information to this paper). As noted, all of the tools were preconfigured on the machine used by the participant to perform the tasks. Each of the tasks in the two sections was assigned in a random order, to minimize the risk of bias entering the study.

6.6.6 Results

Result	Globus Toolkit	AHE CLI	UNICORE GUI	AHE GUI	AHE with Cert	AHE with ACD
Percentage of successful users	45.45	75.76	30.30	96.97	66.67	96.97
Percentage of users satisfied with tool	27.27	53.54	47.47	79.80	51.52	87.88
Percentage of users who found tool difficult to use	45.45	25.25	26.26	5.05	27.27	0.00

Table 1: Summary of statistics collected during usability trials for each tool under comparison.

Our usability tests show very clear differences between the different tools tested, based on the usability metrics defined above. Table 1 presents key measurements from our findings. Due to problems with the delivery platform (such as web browser crashes half way through a set of tests), the results from six participants have been excluded from our results, meaning that the results presented have been gathered from a cohort of 33 participants.

We applied a 1-tailed, paired t-test to our results to determine the statistical significance of any differences between the tools being compared. We compared the Globus command line client with the AHE command line tool, and the UNICORE graphical client with the AHE graphical client. We also compared the AHE using a digital certificate to the AHE using ACD authentication. The P-values of these t-tests are shown in table 2, along with mean scores for the five different metrics. A $p < 0.05$ shows that the difference between the tools is statistically significant.

Our first usability metric looked at whether or not a user could successfully complete the set of tasks with a given tool. Table \ref{tab:results} summarizes the percentage of participants who were able to complete all tasks for each tool. Although the failure data is measured on an ordinal scale (Success, Failed etc.), we have converted it to numerical data in order to more easily compare results. The mean failure rate is shown in table 2, with a lower score meaning there were less failures when using the tool. Also shown in table 2 are the P-value scores; the AHE command line was found to be less failure prone than the Globus command line ($t(33) = 1.41, p < 0.05$), the AHE GUI was found to be less failure prone than the

UNICORE GUI (t(33) = 1.07, p< 0.05) and AHE with ACD was found to be less failure prone than AHE with X.509 certificates (t(33) = 1.03, p < 0.05).

Our second usability metric was a measure of how long it took a user to complete an application run. Figure 1 plots the mean times taken to complete the range of tasks with each tool. Again, the differences are statistically significant as shown in table \ref{tab:ttests}, with participants able to use AHE to run their applications faster than via Globus or UNICORE, and AHE with ACD faster than AHE with X.509 certificates.

Our third usability metric measured user satisfaction with the tools used. In table 1 we have summarized the percentage of participants who reported being either Satisfied or Very Satisfied with a tool. The Likert scale data is again ordinal, but we have converted it to numerical data in order to compare it, according to commonly practice. The mean satisfaction level is reported in table \ref{tab:ttests}, a higher score meaning that a user was more satisfied with the tool. Again, users reported being more satisfied with the AHE than with other tools, and with ACD than with X.509 certificates, as show by the P-value scores table.

Our fourth usability metric looked at how difficult a user perceived a tool to be. Again the percentage of users who found a tool difficult or very difficult is summarized in table 1. The mean difficulty scores are shown in table 2, with a higher score meaning that the tool was perceived as being more difficult to use. The AHE GUI client was perceived as being less difficult to use than the UNICORE GUI client (t(33) = 1.73, p< 0.05), the AHE command line interface was perceived as being less difficult to use than the Globus command line tools (t(33) = 2.55, p < 0.05), and AHE with ACD was perceived as being less difficult than AHE with digital certificates (t(33) = 1.52, p < 0.05).

Our final usability metric measured a participant's overall impression of a tool using the SUS usability scale. The mean SUS score is shown in table 2, with a higher score meaning the tool is more usable. Again, we found statistical significance, with AHE GUI being rated as more usable than the UNICORE GUI, AHE command line being rated higher than Globus, and AHE with ACD being rated higher than AHE with digital certificates, as summarized in table 2.

	Middleware Tests				Security Tests	
	Globus Toolkit	**AHE CLI**	**UNICORE GUI**	**AHE GUI**	**AHE with Cert**	**AHE with ACD**
Mean SUS score. 100=most usable	37.50	51.89	52.95	69.47	51.21	72.12
SUS score *P*–value	6.14821×10^{-4}		2.55007×10^{-4}		1.10235×10^{-7}	
Mean task time (seconds)	667.73	606.18	587.33	388.70	309.00	131.39
Mean task time *P*–value	3.55845×10^{-2}		3.49719×10^{-4}		8.97553×10^{-5}	
Mean failure rate. 5=most failure prone.	2.11	1.41	2.16	1.07	1.45	1.03
Failure rate *P*–value	6.23844×10^{-8}		6.60682×10^{-14}		8.18544×10^{-4}	
Mean perceived difficulty. 5=most difficult	3.15	2.55	2.44	1.73	2.67	1.52
Perceived difficulty *P*–value	7.27699×10^{-7}		3.23194×10^{-7}		2.27949×10^{-5}	
Mean satisfaction. 5=most satisfied	2.68	3.29	3.34	4.05	3.12	4.27
Satisfaction *P*–value	7.27699×10^{-7}		1.28956×10^{-6}		7.50398×10^{-6}	

Table 2: The mean scores and t-test P-values for our five usability metrics, comparing the AHE and Globus command line clients, the AHE and UNICORE graphical clients, and the AHE with and without ACD.

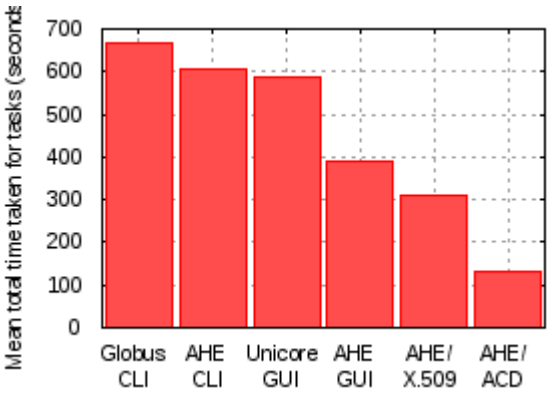


Figure 1: Mean time taken to complete a range of tasks with each tool.

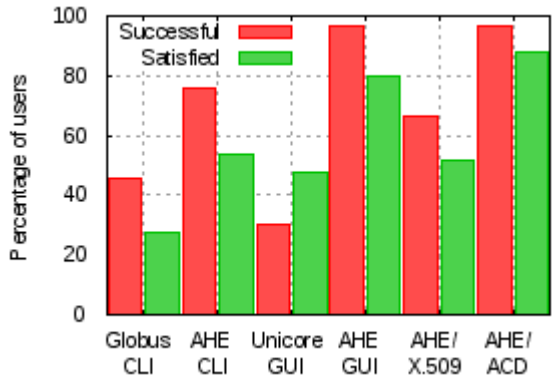


Figure 2: a comparison of the percentage of users who were satisfied with a tool and the percentage who could successfully use that tool.

6.6.7 Discussion of Results

The results presented in the previous section clearly confirm our hypotheses, that the application interaction model used by the AHE is more usable than the resource interaction model implemented in the UNICORE and Globus toolkits, with AHE found to be more usable for each of our defined usability metrics. We believe the reason for this is due to the fact that AHE hides much of the complexity of launching applications from users, meaning that (a) there are less things that can go wrong (hence the lower failure rate) and (b) there are less things for a user to remember when launching an application (hence the higher satisfaction with and lower perceived difficulty of AHE tools). The fact that the AHE model encapsulates input and output data as part of an application's instance (and stages data back and forth on the user's behalf) means that application launching is faster via AHE.

In the case of ACD security, the familiar username and password were clearly found to be more usable than X.509 certificates, but it should also be stressed that the scenario modelled here represented the `best case' scenario, where a user was already given an X.509 certificate with which to configure their client. As previously noted, in the real world a user would have to go through the laborious process of obtaining an X.509 certificate from their certificate authority, which renders the ACD solution far more usable still.

The failure rate when using a tool is dependent on all of the subtasks being completed successfully; if one task failed, it meant that the following tasks could not be successfully completed (marked `Failed due to previous' by the observer). This is, however, analogous to real world scenarios where, for example, a user will not be able to download data from a grid resource if his job is not submitted correctly.

We noted particular problems experienced by participants using the UNICORE middleware, related to staging files and configuring job input files. However, these problems were not noted by the participants themselves, due to the jobs appearing to submit properly. Figure 2

plots the percentage of users reporting satisfaction with a tool alongside the percentage of users who successfully used that tool. Curiously, more users reported satisfaction with the UNICORE client than were able to use it successfully, suggesting that many participants did not realize their jobs had not completed successfully.

The freeform comments made by users of the individual systems also provide some illuminating insights as to their usability. Regarding the use of ACD security with AHE, one participant reported "To deal with security issues a user is much more at ease with a simple username/password system. The use of certificates just complicates the process unnecessarily". Another participant highlighted the problems involved in learning the command line parameters required to use the Globus Toolkit, reporting "there were difficulties in accessing the outside servers i.e. adding gsiftp:// or when to input the whole path into the command line".

7 References

1. JSDL - Fred Brisard, Michel Drescher, Donal Fellows, An Ly, Stephen McGough, Darren Pulsipher, Andreas Savva: Job Submission Description Language (JSDL) Specification, Version 1.0, http://www.gridforum.org/documents/GFD.56.pdf, 2005.
2. HPC-BasicProfile - Blair Dillaway, Marty Humphrey, Chris Smith, Marvin Theimer, Glenn Wasson: HPC Basic Profile, Version 1.0, http://www.ogf.org/documents/GFD.114.pdf, 2007.
3. K. Rycerz, M. Nowak, P. Pierzchala, M. Bubak, E. Ciepiela and D. Harezlak: Comparision of Cloud and Local HPC approach for MUSCLE-based Multiscale Simulations. In Proceedings of The Seventh IEEE International Conference on e-Science Workshops, Stockholm, Sweden, 5-8 December 2011. IEEE Computer Society, Washington, DC, USA, 81-88 (2011).
4. I. Foster,A. Grimshaw,P. Lane,W. Lee,M. Morgan,S. Newhouse,S. Pickles,D. Pulsipher,C. Smith,M. Theimer: OGSA Basic Execution Service, Version 1.0, http://www.ogf.org/documents/GFD.108.pdf, 2008
5. Goodale, T. and Jha, S. and Kaiser, H. and Kielmann, T. and Kleijer, P. and Von Laszewski, G. and Lee, C. and Merzky, A. and Rajic, H. and Shalf, J.: SAGA: A Simple API for Grid Applications. High-level application programming on the Grid. Computational Methods in Science and Technology
6. Fredrik Hedman, Morris Riedel, Phillip Mucci, Gilbert Netzer, Ali Gholami, M. Shahbaz Memon, A. Shiraz Memon, Zeeshan Ali Shah: Benchmarking of Integrated OGSA-BES with the Grid Middleware. Euro-Par Workshops 2008.

7. John Brooke Usability evaluation in industry, SUS—a quick and dirty usability scale (CRC Press, Boca Raton, FL), pp 189–194 (1996).
8. Chang, D.W.; Zasada, S.J.; Coveney P.V.: The Application Hosting Environment 3.0: Simplifying Biomedical Simulations using RESTful Web Services, CBMS 2012 (in press).
9. Groen, D.; Rieder, S.; Grosso, P.; De Laat, C.; Portegies Zwart, S.: A lightweight communication library for distributed computing. Computational Science and Discovery, vol. 3, no. 015002 (2010).