



## D6.2 Report on Best Practices

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## 1 Executive summary

The aim of this deliverable is to report on best practices defined and adopted during the course of the MAPPER project. The deliverable describes the status of the MAPPER services and infrastructure and outlines the progress achieved with respect to collaboration with European infrastructure projects, including EGI and PRACE. Topics covered by this deliverable are expected to evolve over time. As such it is considered to be a living document that will be regularly updated to reflect the latest state of the MAPPER services and infrastructure.

This deliverable reports on best practises in regard to organisation of the MAPPER service activities, deployment and operation of MAPPER services and introduces and describes the EGI-MAPPER-PRACE task force. The task force was established to study, evaluate and provide solutions for integration of multiple IT resources and services operated by European e-Infrastructures. During the first year of the MAPPER project a number of services, including GridSpace, MUSCLE, QCG-Computing, QCG-Notification, QCG-Broker and others, were successfully deployed in the MAPPER research infrastructure. These components are necessary for implementation of the loosely-coupled and tightly-coupled scenarios defined for evaluation of two general classes of multiscale applications.

The EGI-MAPPER-PRACE task force was created with the aim of assessing and implement interoperability models for the European e-Infrastructures based on the use cases defined by the MAPPER project. The task force was formally established during face-to-face meetings between representatives of the EGI, MAPPER and PRACE projects that took place in spring 2011. Following the meeting an MoU between MAPPER and EGI supporting close collaboration between both projects was signed. An MoU between MAPPER and PRACE is being prepared and is expected to be signed later this year.

## **2 Introduction**

The aim of the MAPPER project is to design, implement and operate a distributed research infrastructure based on novel methods for supporting emerging multiscale research projects. To accomplish this goal MAPPER partners should formalize internal practices and study and adopt relevant methods and techniques established in the scientific community. These methods, also called best practices, can improve the overall efficiency of the internal organisation and streamline co-operation and information exchange between MAPPER and collaborating projects.

This document describes standardised best practices that were adopted by MAPPER as well as methods that were formalised and implemented by partners during the course of the project. The practices of interest in the context of the MAPPER services activities cover the areas of documentation, support, service development, integration and deployment as well as operation of the research infrastructure. To facilitate collaboration with European e-Infrastructures MAPPER pays close attention to the practices established by DEISA, EGI, PRACE projects and the National Grid Initiatives (NGIs). For assessment of these practices MAPPER strongly relies on the experience of its partners and public deliverables published by the European e-Infrastructure projects.

The following sections of this deliverable describe the current status of the MAPPER research infrastructure and best practices adopted by the project service activities. The document will be regularly updated to reflect changes in the internal organisation of the project and developments of the infrastructure operated by MAPPER.

## **3 MAPPER Pre-production Infrastructure**

MAPPER services and applications have to pass a thorough testing and validation process before being installed in the MAPPER infrastructure or on European e-Infrastructure resources. The tests have to confirm that the software to be deployed fulfils functional and system requirements and is able to interact with services and the environment the particular software is deployed in. Such interactions include, for instance, runtime characteristics of the service processes, communication with the operating system, drivers and low-level libraries, interoperability with MAPPER services.

To support the service validation process the MAPPER pre-production infrastructure was established. The infrastructure is meant to act as a platform supporting MAPPER service validation and benchmarking activities. The infrastructure is comprised of computing resources provided by the University College London and the German and Polish NGIs. It is accessible to all MAPPER work packages and can thus be used for testing scientific applications. The available resources represent a variety of architectures and platforms, which allows MAPPER partners to prepare services and applications for deployment in the PRACE and EGI environments.

Results of the service validation and benchmarking procedures are recorded and can be shared with collaborating institutions and projects upon request. This procedure introduces minor overhead during the initial service setup process. However it contributes to the minimization of efforts required for subsequent service installation and configuration and helps to optimize communication with external institutions that are interested in deployment of services to support multiscale simulation scenarios.

## **4 MAPPER Service Activities**

The task of the MAPPER service activity work packages, WP4, WP5 and WP6, is to evaluate, test, deploy, operate and verify mutual integration of MAPPER services. The work packages have to ensure that MAPPER services are inline with the project requirements and are able to support execution of multiscale applications in distributed e-Infrastructures. The three work packages have to establish a close contact in order to achieve this goal. As such a number of best practises were adopted to improve the internal structure and communication among the service activities.

Due to the internal organisation and structure of the service activities members of WP4, WP5 and WP6 have to establish and maintain a close contact with each other. Weekly teleconferences are held involving project partners involved in the service activity work packages. This facilitates planning and coordination of work and improves communication and information exchange among project partners. When possible, face-to-face meeting are organised between the members of the work packages. Several such meetings took place over the first year of the project outside of the internal MAPPER, for instance face-to-face, meetings. In overall, it should be notes that this model is working very well what resulted in

substantial achievements of project partners in preparation and deployment of services for the MAPPER research infrastructure and external resource.

Based on the experience of other projects MAPPER has adopted a wiki-based solution for internal documentation, planning and information exchange. The wiki is extensively used by the service activities for coordination of efforts and documentation of completed tasks. Furthermore it offers easy to use yet powerful features that simplify and promote collaboration among project partners.

The service activity work packages have adopted established best practices in the area of service delivery, monitoring and quality assurance. For instance, selected ISO20000 processes are applied for efficient service delivery and change management. These areas are covered in more details in the subsequent sections.

## **4.1 Service Deployment**

One of the primary goals of MAPPER during the first year of the project is to enable, deploy and integrate fast track services that include AHE [19], GridSpace [20] and QCG [1] among others. These services supported by a few deep track components, such as the MUSCLE library, are necessary for evaluation of two selected use cases that represent loosely-coupled and tightly-coupled classes of multiscale applications [18]. The initial efforts were focused on installation and integration of these services in the MAPPER pre-production infrastructure. This was necessary for setting up a distributed environment capable of supporting application activities of WP7 and WP8.

MAPPER services are evaluated and thoroughly tested prior deployment. The evaluation process is performed in an iterative manner. WP4 in collaboration with WP5 prepares the service for deployment by addressing known requirements and issues. Following that WP6 deploys the service on the pre-production resources and reports any detected irregularities to WP4 and WP5. This initiates a new iteration of the evaluation process. Such approach allows us to prepare the components for seamless integration in the existing e-Infrastructures, including EGI and PRACE, minimizing deployment time and guarantying high quality of service provided to the scientific community.

This section covers production services that are deployed on multiple resources. Fast track components that act as centralised services, such as GridSpace, are installed on a single resource and are not covered in this section. Below you will find a description of services that are deployed in the MAPPER infrastructure. These services are currently being deployed on

EGI and PRACE resources in the scope of the EGI-MAPPER-PRACE task force that is described later in this document.

#### **4.1.1 MUSCLE**

The Multiscale Coupling Library and Environment (MUSCLE) is a framework for execution of tightly-coupled multiscale models on distributed resources [16, 17]. The core functionality of the library is implemented in two components: the kernel containing the submodel code and the conduit that provides data transfer functionality. The conduit supports data filters that allow application developers to control submodel data flow. Operations on data that need multiple inputs or multiple outputs but do not qualify as a submodel are called mappers, but are implemented as a kernel.

A MUSCLE model can be executed in a distributed environment by starting a MUSCLE instance on each individual resource or compute node involved in the scenario. Each MUSCLE instance can then be used for executing submodel instances. In such case MUSCLE instances will communicate with each other using the TCP/IP protocol. In situations when a compute resource does not offer a public TCP/IP connection a proxy instance controlling the resource can be set up. When a MUSCLE model is executed, each of the submodels may be started separately. The tightly-coupled scenario is enabled by having loops within the submodels that wait for messages from other submodels at certain points. When no messages are received, for instance if a related submodel unexpectedly quits, the waiting submodel would stop its execution.

The MUSCLE library was deployed on resources that are intended to be used for the tightly-coupled scenario. As a part of the deployment process the available documentation was revised and extended where necessary to satisfy the MAPPER operational model. For instance, a service description form for the MUSCLE library was created. The complete MUSCLE documentation was provided to the selected external resource providers for requirement analysis and deployment of the library.

#### **4.1.2 QosCosGrid**

QosCosGrid [1] is a set of middleware services and tools dedicated for dealing with computationally intensive large-scale, complex and parallel simulations that are often impossible to run within a single computing cluster. With the help of QCG resources distributed across multiple administrative domains may be virtually welded via Internet into



one powerful computing resource. Applications running on top of QCG, in particular the GridSpace toolkit, may transparently use a variety of common technologies, such as OpenMPI [2] or ProActive [3], that are typically used for parallel execution on a single compute resource. Within the MAPPER project, the QosCosGrid stack has been integrated with the MUSCLE coupling library enabling flexible execution of multiscale applications. Since the common multiscale simulations require simultaneous execution, the QCG capabilities for advance-reservations and co-allocation of various types of resources provide a good opportunity to run demanding multiscale scenarios in a distributed environment.

QCG comprises a set of services that are introduced in the following sections. These services provide a basis for MAPPER scenarios. As such, they were deployed on all resources available in the MAPPER per-production infrastructure. Experience collected during installation of QCG components in the heterogeneous MAPPER environment allowed to improve stability and quality of service provided by the components and expand the respective installation and configuration guides.

#### **4.1.2.1 QCG-Computing**

The QCG-Computing service (previously SMOA-Computing) [1] is an open source implementation of SOAP Web Service for multi-user access and policy-based job control routines by various distributed resource management systems (DRMS). It uses the Distributed Resource Management Application API [4] to communicate with the underlying DRMS. The flexible QCG-Computing design and implementation support different plugins and modules for external communication, authentication, authorization as well as interactions with accounting infrastructures and other external services. QCG-Computing service is compliant with the Open Grid Forum HPC Basic Profile [5] specification, which serves as a profile over the job submission description language [6] and the OGSA Basic Execution Service [7]. It offers also remote interface for advance reservations management, and support for basic file transfer mechanisms. Additionally, in order to provide co-allocation support, QCG-Computing may be integrated with QCG-Broker - such a solution is exploited in MAPPER scenarios.

The service was successfully tested with many distributed resources management systems, i.e.: Sun (Oracle) Grid Engine [8], Platform LSF [9], Torque/PBSPRO [10], PBS Pro [11], Condor [12], Apple XGrid [13] and Simple Linux Utility for Resource Management [14]. The Advance Reservations capabilities were exposed for SGE, LSF and Maui [15] (a scheduler that is typically used in conjunction with Torque) systems.

QCG-Computing is one of the core QCG components. It exposes public interfaces to the local resource DRMS and offers capabilities for reservation and job management. The majority of computing scenarios addressed by MAPPER rely on functionalities provided by the QCG-Computing service. As such, one of the goals of the service activities is to guarantee proper operation of the service in a variety of computing environments. To achieve this goal the service activity work packages perform extensive testing and performance benchmarking of the component in the MAPPER pre-production infrastructure. As the infrastructure offers a large number of distinct computing resources we are able to cover many deployment and production scenarios.

#### **4.1.2.2 QCG-Notification**

QCG-Notification is an open source implementation of the family of WS-notification standards (base notification, brokered notification and topics). It supports the topic-based publish/subscribe pattern for the asynchronous message exchange among web services and other involved entities. The main architecture of our system is based on a highly efficient, extended version of the notification broker, managing all items participating in notification events. QCG-Notification offers sophisticated notification capabilities, for example notification message filtering, push and pull messages delivery, and it was successfully integrated with different communication protocols as well as various web services' security mechanisms. The modular architecture of QCG-Notification also provides a great opportunity for developers to build new extensions and plugins to meet other specific requirements.

From the architecture perspective, QCG-Notification exposes a well-defined web service interface corresponding to the role of notification broker as well as it offers other standard interfaces for managing subscriptions and pull points. It supports advanced two-layer notification filtering based on hierarchical topic namespaces and XPath queries on the content of messages.

All functions offered by QCG-Notification can be invoked using different transport protocols. Currently, the system supports the SOAP communication over HTTP, HTTPS, and additionally XMPP. Thanks to the XMPP based communication, all notification parties, namely subscribers, publishers, notification consumers and QCG-Notification itself, can be located behind firewalls with only well defined outgoing TCP/IP port open for the XMPP transport communication.

The QCG-Notification service is similar to QCG-Computing as it has a key role in the MAPPER service stack. As such, the QCG-Notification service undergoes the same rigorous evaluation and quality assurance process as QCG-Computing.

#### **4.1.2.3 QCG-Broker**

QCG-Broker [1] is a meta-scheduling system, which allows developers to build and deploy resource management systems for large scale distributed, multi-cluster computing infrastructures. The main goal of QCG-Broker was to manage the whole process of remote job submission and advance reservation to various batch queuing systems and subsequently to underlying clusters and computational resources. QCG-Broker deals efficiently with various meta-scheduling challenges, e.g., co-allocation, load balancing among clusters, remote job control, file staging support and job migration.

The QCG-Broker service has been designed as an independent component which can take advantage of various low-level core and grid services and existing technologies, such as QCG-Computing or QCG-Notification, as well as various grid middleware services such as gLite, Globus or UNICORE. The XML-based job definition language supported by QCG-Broker is job profile. The job profile schema makes it relatively easy to specify the requirements of large-scale parallel applications together with the complex parallel communication topologies. Consequently, application developers and end users are able to run their experiments in parallel over multiple clusters as well to perform various benchmark-based experiments as alternative topologies are taken into account during meta-scheduling processes in QCG-Broker.

QCG-Broker is a central service that can control multiple resources. It is advised that only one QCG-Broker service is operational in an e-Infrastructure at any given moment in time. As such, the main focus of the MAPPER service activities is to guarantee full functionality of the service on resources that satisfy the service system requirements.

## **4.2 Monitoring and Quality Assurance**

Operational MAPPER services are monitored to ensure their availability and correct functionality. At the current stage monitoring is performed using the Nagios tool [21] deployed at the Leibniz Supercomputing Centre. Nagios is a de-facto standard for monitoring service and application availability in large-scale infrastructures. The tool is used by multiple

e-Infrastructure projects, including EGI. This offers an added benefit as, if necessary, Nagios extensions developed by MAPPER can be easily ported to other e-Infrastructures.

MAPPER services are monitored according to the functional requirements devised by the Technical and Application Boards. During the design process the MAPPER Technical Board considers monitoring requirements and solutions used by other European e-Infrastructures, in particular EGI and PRACE, to ensure that requirements defined within these e-Infrastructures can be easily fulfilled. As mentioned above, the existing MAPPER monitoring infrastructure satisfies EGI requirements. PRACE uses a different collection of monitoring tools that are currently not supported in MAPPER. It is expected that the PRACE requirements will be addressed by service activities in the near future.

The primary goal of the monitoring efforts is to collect information about availability of MAPPER applications and services. Currently WP6 focuses on service-level monitoring verifying operational status of MAPPER services by, for instance, checking whether specific service processes are running and respond to basic queries and requests. Members of MAPPER service and joint research work packages are involved in the monitoring activities by providing feedback and participating in design and development efforts geared towards implementation of new functionality and evaluation of new monitoring technologies.

Incidents, such as service failures, detected by monitoring tools are reported to WP6, which classifies each incident based on its impact on the MAPPER e-Infrastructure and assigns it to the service activities member responsible for the failing component. If the problem cannot be resolved by MAPPER service activities it is escalated to the developers of the respective service. After the incident is resolved, all affected parties are informed and the solution is documented in MAPPER wiki.

Monitoring data collected by MAPPER is archived and can be used for reporting and quality assurance. The availability of MAPPER services is evaluated by the project partners, in particular by the MAPPER Technical Board. The board closely observes service quality levels and the overall availability of the MAPPER e-infrastructure and reacts in cases when service levels fall below defined limits.

### **4.3 Documentation and Support**

Comprehensive documentation for services and applications is crucial for successful operation of MAPPER work packages, especially service and joint research activities.

Therefore an environment able to support collaborative work of multiple activities was necessary. A wiki-based solution was chosen by project partners to address this need. MAPPER wiki acts as a central place for all work packages to publish project relevant documents that should be available to all project partners.

Documents that cover MAPPER infrastructure component, including application and service installation and administration manuals, user guides and tutorials are made available to public via the MAPPER web site. These materials focus on achieving the following goals. First, providing detailed information and guidance to MAPPER users who are willing to run complex multiscale simulations. Furthermore these documents act as a reference for e-Infrastructure operators charged with installation and configuration of MAPPER components on production e-Infrastructures. Documentation of MAPPER services is regularly vided and extended, for instance to address platform specific requirements, as it plays an important role in achieving the sustainability goals of the MAPPER project.

To facilitate the deployment process of all successfully validated software components WP6 designed the MAPPER service description form. The form describes MAPPER application and services and provides their essential characteristics including system and security requirements. The form is filled out prior to the deployment of each service in the MAPPER e-Infrastructure and is provided as a part of the service documentation package. The service description form proved to be a very successful addition to the publicly available service guides. The form greatly improved communication between MAPPER and representatives of the EGI and PRACE e-Infrastructures responsible for deployment of MAPPER services in the context of the EGI-MAPPER-PRACE task force. The form will be made available for each service and included in the respective installation and configuration manual as a part of the project sustainability efforts.

Another aspect to get attention of the MAPPER project is support of the scientific community. MAPPER will operate a help desk and provide VOs and user communities with comprehensive technical support. Reported problems will be handled by the service activities according to the ISO 20000 practices. Issues beyond the expertise of MAPPER will be escalated to external entities, such as application developers or service providers.

## 5 EGI-MAPPER-PRACE Task Force

One of the main goals of WP6 is to ensure interoperability of MAPPER with the existing European e-Infrastructures, such as EGI and PRACE. As MAPPER will not operate its own computing infrastructure, it is vital that designed and developed computational methods, applications and services can be successfully deployed and integrated in the e-Infrastructures available to the European scientific community. To initiate discussion with the EGI and PRACE projects two face-to-face meetings with representatives of the respective projects took place in the first half of 2011. The emphasis of the meetings was a bilateral introduction of the projects and a discussion concerning the possible collaboration. Representatives of both EGI and PRACE projects expressed their great interest in working together with MAPPER. An additional goal outlined for the three projects was to evaluate the interoperability potential between the EGI and PRACE e-Infrastructure using the use cases defined by MAPPER. As an outcome of the meeting the EGI-MAPPER-PRACE task force was formed. The task force includes members of the three projects representing various activities, including operations, development, application enabling and user support.

The work plan for the task force is detailed until the end of 2011 and will be extended later this year. The initial focus of the task force is exchange of information regarding operational practices, services, applications and tools and deployment of MAPPER fast track components, including QCG-Computing, QCG-Notification and MUSCLE, on the production EGI and PRACE resources. Both EGI and PRACE project committed to provide support necessary for successful deployment and operation of the MAPPER components. To formally support these efforts an MoU with EGI was signed in August 2011. An MoU with PRACE is currently being prepared and is expected to be signed later this year.

To facilitate information exchange EGI has setup a wiki environment accessible to all members of the task force. The task force wiki is used as a platform for exchange of practices and experience. It acts as a hub for collection of information describing applications, services and policies relevant to the interests and goals of the task force. For instance, the wiki collects references to documentation of the MAPPER services to be deployed in the e-Infrastructures, as this information is essential for evaluation of the components by the EGI and PRACE representatives. EGI and PRACE user account generation procedures to be followed by the MAPPER members are described in the task force wiki as well.

The loosely- and tightly-coupled scenarios defined by MAPPER assume that MAPPER services are available on the selected EGI and PRACE resources. To achieve that representatives of the e-Infrastructures have to evaluate the services in accordance with the operational policies in force. Details on the missing requirements are communicated to MAPPER that addresses all open issues. For instance, as a part of this effort the work packages four, five and six will be extending the monitoring and accounting functionality of MAPPER services. At this moment MAPPER has a pilot access to Huygens, an HPC system hosted at SARA. The system is used for the development of the loosely- and tightly-coupled scenarios and deployment of fast track services.

## 6 Conclusion

This document outlines best practices defined and adopted by the MAPPER project. Functional areas covered in this document include the MAPPER pre-production infrastructure, deployment and operation of MAPPER services, monitoring, quality assurance, documentation and user support. The EGI-MAPPER-PRACE task force, its structure and goals are introduced in the document. The task force work plan that was describe will be updated beyond year 2011 based on the status and objectives of the task force.

New best practices will be assessed and adopted over the course of the project to satisfy the evolving requirements of the MAPPER e-Infrastructure. Changes and developments in this area will be reflected in the future issues of this deliverable.

## 7 Acronyms and References

### 7.1 Acronyms

AHE	Application Hosting Environment
DEISA	Distributed European Infrastructure for Supercomputing Applications
DRMS	Distributed Resource Management System
EGI	European Grid Initiative
HPC	High Performance Computing
HTTP(S)	Hypertext Transfer Protocol (Secure)
ISO	International Organization for Standardization
MoU	Memorandum of Understanding

MUSCLE	Multiscale Coupling Library and Environment
NGI	National Grid Initiative
OGSA	Open Grid Services Architecture
PRACE	Partnership for Advanced Computing in Europe
QCG	QocCosGrid
SOAP	Simple Object Access Protocol
UNICORE	Uniform Interface to Computing Resources
WP	Work Package
WS	Web Service
XMPP	Extensible Messaging and Presence Protocol

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