D3.1 Report on the policy framework resource providers need to adopt to support the MAPPER Project

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1 Introduction

The MAPPER project aims to enable multiscale computing on production-quality compute, storage and networking infrastructures. Here multiscale computing means doing a large computation by coupling different applications, each of which may operate on a different spatial and/or temporal scale. In MAPPER we plan to allow researchers to run their multiscale simulations across multiple production resources, with each resource handling different aspects of a multiscale simulation. The application of multiscale production simulations to the existing infrastructures requires considerable modifications to the policy frameworks of resource providers such as supercomputer centres and networking organizations. Many of the current frameworks have been developed with a strong emphasis on the resource providers and the committees overseeing them, and have critically unfavourable consequences for the user base (e.g., reduced usability or lack of reliable connectivity). The consequences of these policies are even so far-reaching that many sites have been unable to adopt software and usability advances proposed several years ago or more, such as support for multi-site community schedulers, advance (co-)reservation and single sign-on. This document provides a summary of the shortcomings in the political framework of the production resource providers. Although the policy shortcomings mentioned here are specifically tied to the MAPPER project and its affiliated communities, they also limit the research possibilities of a much wider range of user communities. If left unresolved, these policy shortcomings will impair the research work of an even wider range of user communities in the coming years, as users will be required to construct ad-hoc workarounds to resolve policy shortcomings, to reduce the resolutions of their simulations and adopt a smaller but more facilitating infrastructure (such as a grid of locally owned PCs) or to rely on commercial implementations of cloud computing schemas to conduct public research.

2 Overview of the stakeholders involved

Before we present the policy framework itself, we will identify the stakeholders within the context of this framework. As with any political development, there are different groups which either have decision power over these policies, or are affected by them in one way or another. These stakeholders may have differing needs and priorities, which could lead to a political deadlock in cases where these needs and priorities heavily conflict. Within the context of MAPPER in general, and the policy framework for resource providers in specific, we distinguish the following types of stakeholders:

- Users and user organisations
- Resource and tool providers
- Information and Communication Technology (ICT) developers

- Administrators
- National research and education networks (NRENs)
- Policy bodies and policy makers
- National and international funding agencies

Below we provide a brief description of each type of stakeholders and its specific needs. We provide a list of the concrete stakeholder organisations and contact persons in Appendix 2.

Users and user organisations (US). This group consists of researchers in academia or industry who wish to perform scientific simulations on large-scale production resources. These resources include, but are not limited to, instruments, computational power, storage capacity and high-quality network connections. However, the resources provided may require certain software tools or policy constraints to fullfill the goals of the users. Researchers do not necessarily operate in isolation, and commonly band together into scientific projects or even virtual communities. Such projects or virtual communities provide a uniform political interface between the users and the other stakeholders, eliminating some degree of complexity from political negotiations. *Needs:*

- Resources and resource allocations to use for their scientific simulations.
- Software tools to provide required functionalities for their scientific simulations. Policies that allow them to use the resources as they intend.
- Interoperability and connectivity between resources to enable them to use more than one site.
- Minimizing bureaucratic overhead when requesting allocations and constructing/executing their simulations.

Resource and tool providers (RP) The computational, storage and network resources, as well as some of the software tools required by the users are owned by resource providers. These providers possess a limited set of resources, which they wish to put to optimal use. The resource providers addressed in this deliverable have all agreed to participate in facilitating scientific simulations, i.e. help put the scientific simulation plans of researchers into practice. However, the extent of their efforts to facilitate scientific simulations are constrained by efficiency requirements from funding bodies, as well as their needs to facilitate other classes of applications. *Needs:*

- Ensure appropriate usage of their resources to justify the existence and funding of these resources.
- Facilitate the use of their resources for scientific simulations.
- Facilitate the use of their resources for applications other than scientific simulations.

- Minimal management overhead of their resources (e.g., by discouraging intrusive software from being installed).
- Adhere at all times to the national non-proliferation and privacy laws.
- Ensure that the security of the resources does not get compromised at anytime.

ICT developers (DEV) Large-scale production resources are frequently under-equipped to run specific scientific simulations, and require the installation of additional software to make scientific simulations possible as intended by the users. This additional software may be readily available, or may have to be developed for this particular purpose. The ICT developers are stakeholders that seek to push the functionality of supporting software such as middleware services or user-driven software tools, in part to facilitate existing users and in part to encourage new users to adopt their ICT solutions. *Needs:*

- Maximal functionality of their developed software.
- Facilitating their users by improving and deploying their software.
- Increase user base and exposure for their developed software.

Administrators (ADM) While RPs own resources and tools and users "consume" resources, administrators are responsible for enabling both the correct access to the resources and the availability of the resources while adhering to RP specific policies and/or virtual community policies. *Needs:*

- Ensuring the dependability of resources (availability, reliability, etc).
- Ensuring the authorized access to resources.
- Ensuring the resources are maintained correctly.

National research and education networks (NRENs) An NREN is responsible, on a national basis, for the provision of data communications networks and services to the research and education community of its country. The NREN network typically connects other networks at regional or metropolitan level. NRENs in Europe cooperate together and provide the access to European wide networking infrastructure operated by DANTE [11]. DANTE provides the data communications infrastructure essential to the development of the global research community, and is coordinating joint research and development activities in the GEANT3 project [12]. The focus of GEANT3 lies strongly on the provisioning of network connections. *Needs:*

- Appropriate usage of their resources to justify the existence and funding of the networks.
- Avoiding the fragmentation of security between different organizational domains.

- In time: introduce new protocols to achieve better network throughputs on the networks.

Policy bodies and policy makers (PM) The policy bodies and policy makers are the focal point of this deliverable. These include people working for resource providers who decide on policy matters, as well as organisations such as PRACE or GEANT which prescribe certain policies for multiple resource providers. The policy makers are required to assess the needs and priorities of all the stake holders, and introduce policies to ensure that these needs are met as much as possible. This process is straightforward in principle, though there are several complicating factors. For example, the needs of different groups may conflict or the policy deemed optimal may impose a major change on the current state of affairs, and requires considerable effort and funding to implement. *Needs:*

- Information on the needs and priorities of other stakeholders.
- Minimization of conflicting needs, which makes it more difficult to propose fully effective policies.
- Information on the effect of implementing candidate policies.

National and international funding agencies (FA) National and international funding agencies provide funding in many cases to resource providers, users and ICT developers. They are responsible for accepting proposals and funding projects and infrastructure. Because of this, their validation and quality assurance methods may have an effect on the needs of the other (funded) stakeholders. *Needs:*

- Means to verify that funding is used as intended.
- Means to validate the quality and effectiveness of the funded research/facilities.
- Ensuring that RPs are aligned to support the research projects that they fund.

2.1 Conflicting needs

This section briefly describes some of the aforementioned needs which may conflict with each other. Solutions for these conflicts in areas relevant to MAPPER are proposed in the policy framework.

Required user functionality (US) vs. maximized resource usage (RP) Resource providers have applied software and policies to maximize the load of their resources. However, modern scientific simulations which encompass multiple scales require an orchestrated use of a wide range of computational and network resources. Orchestrating and co-allocating different resources becomes more difficult when the load on these resources is high. Yet facilitating these modern scientific simulations might warrant a decrease in average load on the resources.

Ease of access (US) vs. security and adherence to laws (RP, PM). Users prefer to have easy and convenient access to individual resources, and be able to switch between different resources or use multiple resources without additional administrative overhead. However, RPs face a number of constraints which can make the process of gaining access to resources a more heavyweight process. They are often unable to build up a personal trust relationship with individual researchers, as these researchers may reside in different countries. Furthermore, they have to abide the National and European laws for privacy and non-proliferation, which also apply to computing infrastructures. A third constraint is the RPs need to keep the resources secured from the outside world. Unauthorised access may result in abuse of the facilities and contractual penalties, and should be prevented in all cases.

Minimal management overhead (RP) vs. maximal software functionality (DEV) ICT developers wish to push the functionality of their software to better accommodate the needs of the users. However, the addition of functionalities over time tends to result in more heavyweight software stacks, which are more difficult to install and maintain and may even require administrative privileges. This side effect of more functional software conflicts with the needs of Resource Providers to minimize their management overhead, and to limit the number of software tools which need to be installed using administrative privileges.

3 Policy framework

The framework proposed in this document consists of two sections. The first section contains the fast track policy requirements, which are the requirements for supporting the fast track components of MAPPER. These requirements are crucial for the rapid deployment of the MAPPER scenarios and need to be implemented as soon as possible. The second section contains the deep track policy requirements, which are the requirements for supporting tightly-coupled multiscale simulations and to achieve a production-level quality of service. The deep track policy changes need to be put into place before the deep track components are deployed to ensure a smooth rollout of the deep track scenarios further into the project. For each item we describe the current prevailing situation, and the desired policy environment.

3.1 Fast Track Policy Requirements for MAPPER

Obtaining Compute Time and Storage Space

These requirements relate to the procedures used to acquire compute time and storage space on e-infrastructures.

Scope of policy: Global, applies to PRACE, EGI, network providers and data storage providers.

MAPPER is an EU project aiming to bring distributed multi-scale applications to European e-infrastructures, yet at this time the existence of an EU project alone does not grant any right to any compute time. We are currently required to write separate proposals to obtain time on any major computing facility within Europe, or use time slices of existing allocations which were requested for different projects. Although we must admit requirements by RP and ADM, the need for additional proposals within the context of an existing EU project significantly increases the bureaucratic burden, as multiple proposals are written and reviewed for the same project. In addition, part of the project proposals may be rejected, requiring the project participants to either write more proposals or allowing the project to remain uncompleted. Furthermore, the calls for computing and storage allocations are made in complete ignorance of the aims and requirements of these projects, with obvious consequences (bids will likely be unsuccessful).

To reduce the bureaucratic overhead of EU projects in general, and MAPPER in particular, the procedure of requesting compute time and storage must be greatly streamlined. This can be accomplished by including requests for compute time and storage space in EU project proposals. A review commission consisting of FAs and RPs can then judge the scientific potential and computational demands of the project, and decide whether the overall project qualifies for funding. If the project does qualify, the required budgets for funding, computing and storage can then all be awarded to the project. This procedure eliminates the need for researchers to write multiple proposals for a single project, and prevents projects from receiving a financial budget for research, but not the required computing and storage allocations.

Resource Scheduling

These requirements relate to the procedures used to schedule jobs on computational resources. It includes aspects such as advance reservation and prioritized access (urgent computing).

Scope of policy: Site-specific, applies to all supercomputing centres involved or Global.

Multi-scale applications generally use multiple computational sites, running across these sites either concurrently or changing active sites during runtime. However, different computational sites are only rarely available at the same time, preventing users from using the resources concurrently. To make multi-scale applications possible at all, we therefore require to reserve the required resources on all sites in advance. Using advance reservation, we are then able to synchronize the different simulations running on different resources. Advance reservation is also crucial to simulations hat use real-time visualization (e.g., blood flow simulations used to assist a medical decision) or computational steering. There are a large number of production-quality advance reservation systems available today, some of which also support reservations across sites (e.g., the Highly Available Resource Co-allocator [1] and the QosCosGrid Brokering System [2]).

In addition, several simulations within the scientific community in general, and the MAPPER project in particular, only produce useful results when they are completed in time. These range from disaster-prediction simulations, such as weather simulations or forest fire simulations, to simulations which serve to assist doctors in their medical procedures, such as arterial blood flow simulations. An application will need to run with exceptional priority (using Urgent Computing), bypassing the regular scheduling queue and sometimes even requiring the cancellation of existing simulations, in order to complete in time. The scheduling policies of existing supercomputers generally do not support urgent computing at the moment.

The MAPPER project requires policies from the RPs which make advance reservations on their resources possible – but over writable when urgent computing access is required. This applies both to compute infrastructures, as well as wide area network connections. Urgent computing middleware is already in existence (e.g. SPRUCE [5]), and the MAPPER project requires urgent computing, as well as several projects which are part of MAPPER (e.g., the Virtual Physiological Human). In the short term, we absolutely require policies that support advance reservation in any way, but to structurally facilitate advance reservation and urgent computing we will need to reach a political agreement with resource providers. This agreement then defines the terms and conditions under which the RPs are willing to support advance reservation and urgent computing. The support for these policies can be arranged per site but is preferably arranged globally through international infrastructure organizations (e.g., PRACE and EGI).

Connectivity Policies (fast)

These requirements relate to the procedures used to obtain connectivity between computational resources.

Scope of policy: Global, applies to PRACE, EGI, GEANT, DANTE and NRENs.

The connectivity between sites is an essential component in distributed multi-scale simulations. However, it is largely unclear how a user can obtain such connections between sites or gain access to production networks. Gigabit (or 10Gbit) networks may offer the performance required for large multi-scale simulations, but reserving them is a labour-intensive political procedure that may take several months or more which is definitely too long.

The reservation procedure for light paths or other high-throughput should in the very least be streamlined, and agreements should be reached about the terms via which a network reservation can take effect. However, the participating sites should be connected with both a shared network and a dedicated network, the latter being easily reservable using for example a network resource broker or a network reservation system.

Accessing Resources / Usability

These requirements relate to the policies that define sign-on and authentication procedures.

Scope of policy: Global, applies to PRACE, EGI and data storage providers.

Many access policies are determined on a per-site basis, yet MAPPER applications are expected to use multiple sites during their execution. This makes the procedure of accessing a combined infrastructure needlessly complicated. The single sign-on policy is widely adopted through the use of grid certificates, and comes a long way to streamlining this process. However, the process of requesting grid certificates is still far too complicated, and is a known impediment to usage [14], [15].

By allowing research groups to do their work using a group certificate in conjunction with Audited Credential Delegation [3], we can move the overhead of managing grid certificates from the user to the local administrator, and remove one of the largest obstacles for grid accessibility. In addition, Audited Credential Delegation can be used to set up Virtual Organisations.

Interoperability

These requirements relate to the policies that define support for interoperability between resources.

Scope of policy: Global, applies to PRACE, EGI.

The middleware stacks of different sites still have crucial differences in their composition and configuration, which limit the interoperability between sites (even within the same infrastructure [4]!) and add unnecessary obstacles to the deployment of distributed applications. In addition, although a number of standards have been developed for resource access and distributed computing (e.g., DRMAA 2.0) these have not yet been widely adopted by RPs.

Additionally, in the MAPPER project it is possible to adopt standard based interfaces using OGFHPC Profile as well as a set of libraries to get access to different middleware services, in particular gLite, Unicore, GRIA, or Globus via Vine Toolkit [9] and SAGA [10]. Higher level services, in particular those responsible for co-allocation of computational and networking resources, can use the APIs offered by Vine Toolkit and SAGA.

RPs should strive for either a uniform stack of middleware and low-level software tools or a completely uniform interface to use these. Doing so is required to achieve interoperability between different compute resources and infrastructures. In addition, we require policies which ensure that job submissions originating from outside the local site are possible. Also, the development of interoperable middleware can be accelerated if RPs use standards-compliant software stacks for resource access and usage.

Reliability of computing infrastructures

These requirements relate to the policies that define the assurance of resource reliability and cycle refund conditions.

Scope of policy: Global, applies to PRACE, EGI, networking providers and data storage providers.

Essential factors in successfully running any application are the availability and the reliability of computing, networking and storage systems involved. When using distributed infrastructures the availability/reliability requirement becomes tighter, because every site and wide area network link involved is effectively a single point of failure. However, while allocated hours are often refunded for node failures in a single machine run, there are no refund policies for machine failures in projects that use multiple of them.

When the impact of site and network failures in distributed applications propagate to the full application, and lead to a global breakdown, resource providers should not only refund the hours spent on the crashing site by the application, but the hours spent on the other sites directly involved in execution as well.

3.2 Deep Track Policy Requirements for MAPPER

Advance co-reservation

These requirements relate to the procedures used to obtain resource access at a predefined moment in time.

Scope of policy: Global, applies to PRACE, EGI and network providers.

The more advanced multi-scale applications within MAPPER will require an advance reservation system that reserves resources across sites, and is able to extend or request reservations on an automatic basis. The reason for this functionality is to optimally synchronize the runtime of the simulations with the duration of the reservations, and thereby prevent resources from idling. With many sites not yet supporting advance reservation at all, it may currently be difficult to incorporate policies for advance co-reservation. However, a smoothly operating and automated co-reservation system will benefit both the user and the RPs by eliminating the idle time of reserved nodes.

Advance co-reservation tools will require access to the reservation systems of individual sites. To efficiently support these tools, international organizations such as PRACE and EGI will need to adopt policies to ensure a uniform access interface to local reservation systems. This interface can then be used by co-reservation tools such as the QCG broker or HARC. The reservation of network paths will need to be included in this framework as several MAPPER applications will transport large amounts of data between sites. In compensation for this functionality resource providers could adjust their tariffs so that these "advanced users pay more per unit of computing time.

Connectivity policies (deep)

These requirements relate to the procedures used to obtain connectivity between computational resources.

Scope of policy: Both Site-specific and Global (applies to PRACE, EGI and network providers).

Multi-scale simulations require high-quality connectivity between sites, as the performance of these simulations strongly depends on the available bandwidth between sites and the quality of service provided on wide area networks. However, the security policies of especially larger supercomputer centres force users to either use indirect communication methods which reduce the communication performance, or to forego connectivity to the outside world altogether. As a result, projects that use distributed (super)computing are either greatly delayed ([6],[4]) or in the worst case abandoned altogether due to lack of performance ([7]).

Additionally, multi-scale applications require performance measuring and monitoring features for high-quality long distance connections. Developed under the GEANT3 project perfSONAR MDM services allow users to access network performance metrics and perform network monitoring actions across multiple domains, ensuring that any source of congestion or outage on a point-to-point connection can be quickly and easily identified and addressed [12].

Site-specific: To accommodate the MAPPER project, a computational site should allow some means for workflow agents and other multi-scale management tools that reside off-site to connect to the local simulation (e.g. by allowing simulations to connect to the outside world under certain conditions). Global: In addition a reservation policy for network connections (including the end-point nodes) is required to deliver a consistent quality of service to the application users.

Allocation management policies

These requirements relate to the procedures used to publish allocation information with users.

Scope of policy: Global, applies to PRACE, EGI.

Due to the distributed nature of MAPPER applications, the administration of provided and used allocations such as CPU hours or storage space spans across multiple sites, and even multiple infrastructures. Inquiring about available allocations currently has to be done separately for each infrastructure, and in some cases even for each site.

A uniform interface policy to access allocation monitoring tools will greatly streamline the allocation management for MAPPER users, as we can then use local software clients to access and obtain all relevant allocation information in one step. Aside from the obvious improvement in usability, this will also make the users more directly aware of their available hours and storage on the sites involved in MAPPER, and prevent them from unknowingly exceeding their allocations.

Globally Supported Urgent Computing

These requirements relate to the policies towards supporting urgent computing on the full production infrastructure.

Scope of policy: Global, applies to PRACE, EGI.

See the Fast track entry on Urgent Computing I for the rationale behind urgent computing.

Support for urgent computing should be part of the policy framework of international computing infrastructure organizations such as PRACE and EGI, once the technology has been successfully supported by several supercomputing sites.

Appendix I: Project Summary

Today scientists and engineers are commonly faced with the challenge of modelling, predicting and controlling multiscale systems which cross scientific disciplines and where several processes acting at different scales coexist and interact. Such multidisciplinary multiscale models, when simulated in three dimensions, require large scale and indeed frequently extreme scale computing capabilities. The MAPPER project develops computational strategies, software and services for distributed multiscale simulations across disciplines, exploiting existing and evolving European e-infrastructure.

Driven by seven applications from five representative scientific domains (fusion, clinical decision making, systems biology, nano science, engineering), MAPPER deploys a computational science environment for distributed multiscale computing on and across European e-infrastructures. By taking advantage of existing software and services, as delivered by EU and national projects, MAPPER will result in high quality components for today's e-infrastructures. We develop tools, software and services that permit loosely and tightly coupled multiscale computing in a user friendly and transparent way. We integrate our applications into the MAPPER environment, and demonstrate their enhanced capabilities.

The MAPPER project encompasses several types of workflow:

- **Loosely Coupled Multi-scale Simulations**

Multi-scale simulations where the simulation codes are coupled together in a non-cyclic dependency graph and require only one-way exchanges between a given two codes within the simulation.

- **Ensemble Simulations**

These are simulations where multiple instances of the same code runs. The instances run with slightly different parameters and periodically interact with each other. The goal of these simulations is to provide a sample distribution of the final outcome based on these instances, thereby obtaining a more accurate result. Ensemble simulations should be considered as a subclass of loosely coupled multi-scale simulations.

- **Tightly Coupled Multi-scale Simulations**

Multi-scale simulations where the simulation codes are interdependent of each other, resulting in a (partially) cyclic dependency graph. These simulations require two-way exchanges between the codes, and need several codes to be running concurrently or in alternate succession, each of which may use multiple cores.

- **Replica-exchange Simulations**

Coupled simulations which interact with each other, but do not operate on different scales. These simulations would be used, for example, to explore two aspects of a single-scale problem using two different simulation codes. Replica-exchange simulations are categorized as tightly coupled within MAPPER (i.e. with two-way dependencies).

Appendix II: Resource providers considered in this framework

Computing Organizations:

- International: PRACE, EGI**.**
- National: TeraGrid, NGS, BigGrid, Polish Grid, D-Grid.
- Petascale centres: e.g., ALCF (Intrepid), FZJ (JUGENE), NICS (Kraken), PSC (Bulldog), TACC(Ranger), LRZ**.**
- Sub-petascale centres: e.g., SARA, LRZ, EPCC.

Networking Organisations:

- International: e.g., GEANT.
- National: e.g., SURFnet, JANET.
- Data Storage Providers: e.g., various supercomputer centres, UCL's ResearchData@UCL project, the EBI and potentially the EUDAT consortium.

Points Of Contact:

Computing

- Ilya Saverchenko (LRZ, Munich, DEISA/PRACE)
- Dieter Kranzlmuller (LMU, Munich, DEISA/PRACE)
- Arndt Bode (TUM, Munich, DEISA/PRACE)
- Sergiu Sanielevici , Dan Katz (TeraGrid) [8]
- Vincent Breton (EGEE/EGI)
- Walter Lioen (SARA, Amsterdam)
- Gavin Pringle (EPCC, Edinburgh)

Networking

- Richard Hughes-Jones, (DANTE, Cambridge, GEANT key contact)
- Artur Binczewski, (PSNC, PIONIER network)
- Gavin McLachlan (UCL, London)
- Cees de Laat (UvA, Amsterdam)

Data Storage

- Mark van der Sanden (SARA, Amsterdam)
- Andrew Richards (UCL, London)

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