DISTRIBUTED RESEARCH INFRASTRUCTURE FOR HYDRO-METEOROLOGY TO UNITED STATES OF AMERICA

D2.4: Future Integration Report

Abstract: In the context of a sustainable international research infrastructure this document describes the main technical challenges that should be taken into account for future designs of interoperable and integrated transcontinental e-infrastructures. The report also contributes to the project's sustainability plan.

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1 Executive Summary

The objectives of Work Package (WP) 2 (Architecture Harmonization Analysis and Planning) are aiming at assessing the architectures supporting the technologies of present e-infrastructure approaches for Hydro-Meteorological Research (HMR) in Europe and the US with respect to future interoperation and integration. Hence, WP 2 deals with the sustainability aspects of international research e-infrastructures for HMR from both a technical and an organizational perspective. The first objective of WP 2 is to elicit research infrastructure needs and to identify opportunities in fulfilling these needs. The second objective is to propose technical elements and a post project organizational setup for further "pushing" HMR e-infrastructures to sustainably facilitate innovative HMR science.

In this report we outline a rough future integration plan (also called "roadmap") to establish a "unified" HMR e-infrastructure. The plan is based on three ingredients: the organizational part of the DRIHM2US sustainability plan [6] (provided by WP 5), the gaps identified in previous reports D2.1 – D2.3, and a set of interoperability patterns as they exhibit in e-infrastructures in general and in Grid environments in particular.

2 Introduction

The objectives of Work Package (WP) 2 (Architecture Harmonization Analysis and Planning) are related to a sustainable "unified" international research infrastructure, in concreto to the building blocks of an integrated (or at least interoperable) EU/US Earth Science platform [1]. The first objective of this WP is therefore to elicit and prioritize research infrastructure needs, and to identify opportunities in fulfilling these needs. The second objective of this work package is to propose a post project organizational setup and an integration plan for further "pushing" HMR e-infrastructures to facilitate innovative science. This report glues both tasks. In deliverables D2.1 [2], D2.2 [4], and D2.3 [5] we investigated the first objective in more detail. In deliverable D5.2 [6] we assessed organizational options – the second objective. This deliverable combines both aspects by discussing aspects of future planning and integration of

technical components to close the gaps while at the same time adhereing to the sustainability options as outlined in [6].

As a result we propose a rough future integration plan for a unified HMR e-infrastructure consisting of geographically dispersed heterogeneous resources and services (section 6). The plan takes into account the sustainability plan (section 3), the gaps identified in complementary reports (section 4), and interoperability patterns identified in general infrastructures and in HMR e-infrastructures in particular (section 5).

3 Sustainability Approach

The declared goal of DRIHM2US is to sustainably facilitate a more systematic approach to developing, deploying and executing scientific HMR applications across geographies over emerging and future e-infrastructures [1]. Key to the success of the DRIHM2US project is therefore the identification of a set of mechanisms to ensure the sustainability of developed technologies and best practices beyond the lifetime of the project. Approaching this challenge we used in [6] the concept of a sustainability matrix. Figure 1 shows the dimensions of the matrix.

The goal of the matrix is to provide a stringent classification scheme for subsequent assessments of both technology elements and organizational setups. The matrix rows indicate different aspects of science and engineering, both in computer science (ICT R&D, software, resources) and in HMR (science). The columns indicate tasks and activities to support these aspects.

From the matrix we derived requirements and implementation options for a sustainable organisational setup. Methodologically, we applied transformation rules to map the matrix onto organizational specifications. Every matrix cell was assigned one or more structural elements, every such element was associated one or more processes.

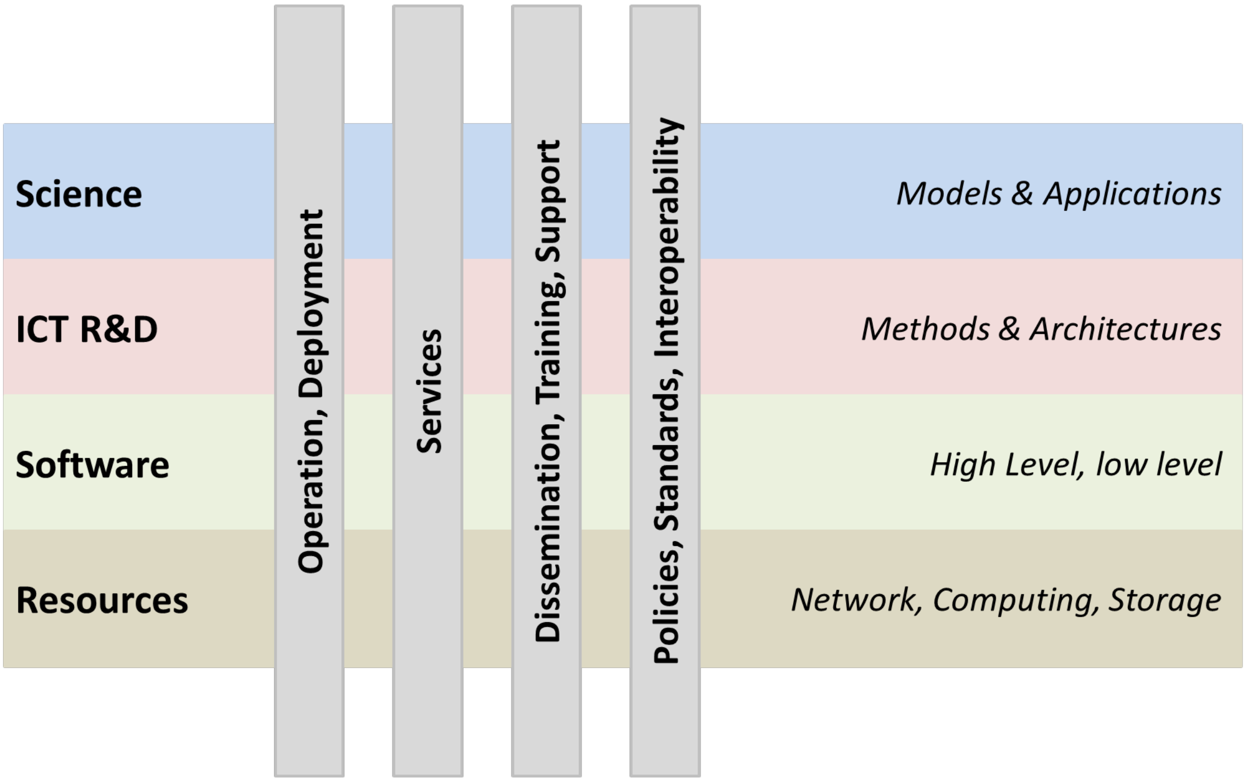

Figure 1: DRIHM2US Sustainability Matrix [6]

The matrix's assessment led to recommendations for both an organizational setup and a technical setup including a basic HMR profile to claim conformance with. We repeat here from [6].

Recommendations for an organization setup

- Use Option VO as the major guideline.
- Outsource the "ICT Operation" to Resource Providers under an a Central/Real organizational option.
- Run the "Education branch" under the Distributed/Real organizational option.
- Assign duties to all participants in the VO option to support other fields of interest. Sign appropriate MoUs and SLAs.

- Assign special task forces (as a "second level VO option") for crowd funding and define appropriate bylaws.

Recommendations for technical elements

- Provide mechanisms for automated configuration, deployment, and execution of HMR simulations across model pools in multi-physics environments.
- Provide mechanisms for dynamic deployment on best suited infrastructures.
- Provide mechanisms for seamlessly integrating mass data.
- Provide mechanisms for real time support.
- Prepare non-trivial demo cases.
- Provide and adhere to standards.
- Implement the HMR Basic Profile.

4 Summary of Gaps

Based on a common architecture model for HMR e-infrastructures and typical HMR scientific use cases we could identify several gaps [4] which we repeat here for convenience (the sequence does not imply any order of importance). Note how these gaps correlate with the recommendations from section 3.

- ability to easily access HM data repositories, models and computing resources
- facilitation of collaboration between meteorologists, hydrologists and Earth Science experts
- easy (and fool-proved) addition of new application components (e.g., models) to existing scientific workflows
- standardized graphical user interfaces (GUI) (including virtual reality integration)
- unified integrated modelling platforms
- dynamic integration of different simulation components in a way that will allow more accurate modelling and prediction of hydro meteorological phenomena
- integration of privately operated meteorological stations
- easy, secure and consistent access to ICT infrastructures (like Grid portals and science gateways) which have to be tailored to the expected user communities
- orchestration of simulation components by coupling appropriate models on various scales using standardized interfaces
- execution of designed experiments on resources typically unknown in advance
- data brokerage

- workflow interoperability solutions to allow workflow sharing
- allow HMR models to interact with each other during the execution of the simulation (tight coupling)
- split large and often unmanageable applications into sets of linkable components which solve singular problems

Additionally, we recommended in [4]

- to form a new role in terms of integrated modelling ('model integrators' or 'curators') whose expertise leads to evaluating valid combinations of models and the issues which will arise in the use of the combination.
- to formally distinguish between roles: When models are used as commodity tools (knowledge encapsulators) the end user may simply require 'the answer', but when models are used for hypothesis testing the end user is the modeller testing the hypothesis. Distinguishing these allows model frameworks to be tailored appropriately for these (and any other) valid uses.
- to provide controlled vocabularies: The assumption that they will all use the English language may be disenfranchising non-English speakers.
- to integrate more intelligence into integrated modelling systems, leading the user into the best courses of action for their use case. For example, different competing models will have different strengths and weaknesses: better results at the equator, better results at the poles; a high sensitivity to incomplete supporting data, a low sensitivity to incomplete supporting data.
- to standardize more and faster: As standards tend to operate at component interfaces, it is desirable that implementing any standard should minimise its intrusiveness to each component. This can be solved at two levels, the library level and the object level. If this lack of intrusiveness is achieved then technology can be exported across technical domains such as inserting the computational core of a numerical model into a game engine. On the other hand, standardization processes tend to be too slow. We have to find ways for acceleration.

5 Challenges of Interoperability

An important aspect of future integration of trans-continental e-science infrastructures (e-infrastructures) is their potential interoperability (or more precisely: the interoperability of components of such infrastructures).

While today HMR scientists regard computational techniques as a third pillar alongside experiment and theory as already shown by the DRIHMS project[1] [7], e-science evolved in the last couple of years as the "global collaboration in key areas of science and the next generation

[1] http://www.drihms.eu/

infrastructure that will enable it."[2] This definition includes HPC silos, high throughput clusters, Grids, Clouds, and many more. Although we focus in this report on Grids as the main e-infrastructure, we explicitly do not exclude the other instantiations. As they all share the common goal of developing future problem solving infrastructures that enables scientific innovations through data, knowledge, and (dynamic) resource sharing via high performance interconnections, it is obvious how to extend our argumentation to integrate these.

Over the years, various types of e-infrastructures evolved that can be classified into different categories according to their services in general and their offered resource-types in particular. The categories are: HPC-driven infrastructures to enable massively parallel applications (examples: parts of XSEDE, PRACE); HTC-driven infrastructures for farming jobs (a.k.a. embarassingly parallel jobs) (examples: EGI, OSG); and hybrid infrastructures with access to a limited set of large-scale facilities while still providing also access to smaller clusters (example: most NGIs). While in theory clear boundaries are hard to define, in practice, however, the boundaries and scopes of these categories are fundamentally different. This results in the well-known set of world-wide non-interoperable Grid islands – typically funded through public sources (examples: EGI and PRACE are funded by the European Commission, XSEDE and the NGIs are funded nationally).

Also typically, each e-infrastructure runs its own technology. Even within one category, different middleware technologies exist. Some use Globus (parts of XSEDE), others use Unicore (parts of XSEDE, PRACE), again others use gLite (EGI) or ARC (NorduGrid) – often in parallel, and often not interoperable. As a result, the state-of-the-art e-infrastructures struggle to provide HMR scientists with a stable and interoperable technology.

On the other hand, infrastructure interoperability is a rather vague term. However, it can be narrowed by observing some advantages of interoperability and resulting requirements:

[2] John Taylor, http://www.nesc.ac.uk/nesc/define.html

- It enables the access to a broader variety of resources of both HPC and HTC type.
- It facilitates extending the functionality of specific infrastructures.
- It allows for enhanced resource utilization as shown in [8] by better load balancing between different kinds of computing infrastructures and their resources.
- It allows for combining resources of different infrastructures in order to realize more realistic HMR simulation chains [7].
- Interoperability requires
    - single-sign on to enable e-scientists to use only one credential in order to access different infrastructures
    - a common agreement on usage policies
    - a job management approach which is able to cope with different job types, job descriptions, and execution environments.
    - mechanisms to cover data transfer, data access, and access to digital repositories and databases.

Following [9], there are several approaches to achieve interoperability between e-infrastructures.

Additional Layer

The most common approach to achieve interoperability is by introducing a separate layer on top of different Grid technologies (i.e. Grid middleware) which holds the required transformation logic (see Figure 2).

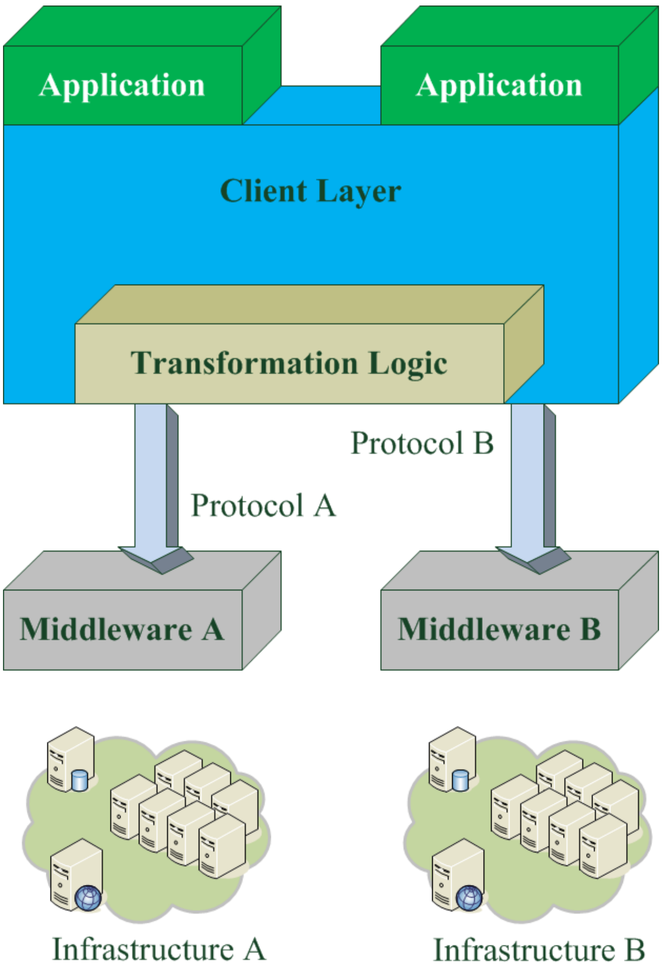

Figure 2: Additional Layer Approach

The transformation logic is responsible for changing job description formats and protocols as required by the respective middleware. This approach is often implemented in portals or APIs and the transformation logic is typically located at clients.

Neutral Bridge

The idea of the bridge approach is to introduce a neutral protocol that can always be used by clients since it is agnostic to changes in a Grid middleware. This neutral protocol is used to contact the neutral bridge implementation which in turn uses its transformation logic to adapt

the neutral protocol to the different proprietary formats for each corresponding Grid middleware (see Figure 3). This approach is taken by the Globus Toolkit.

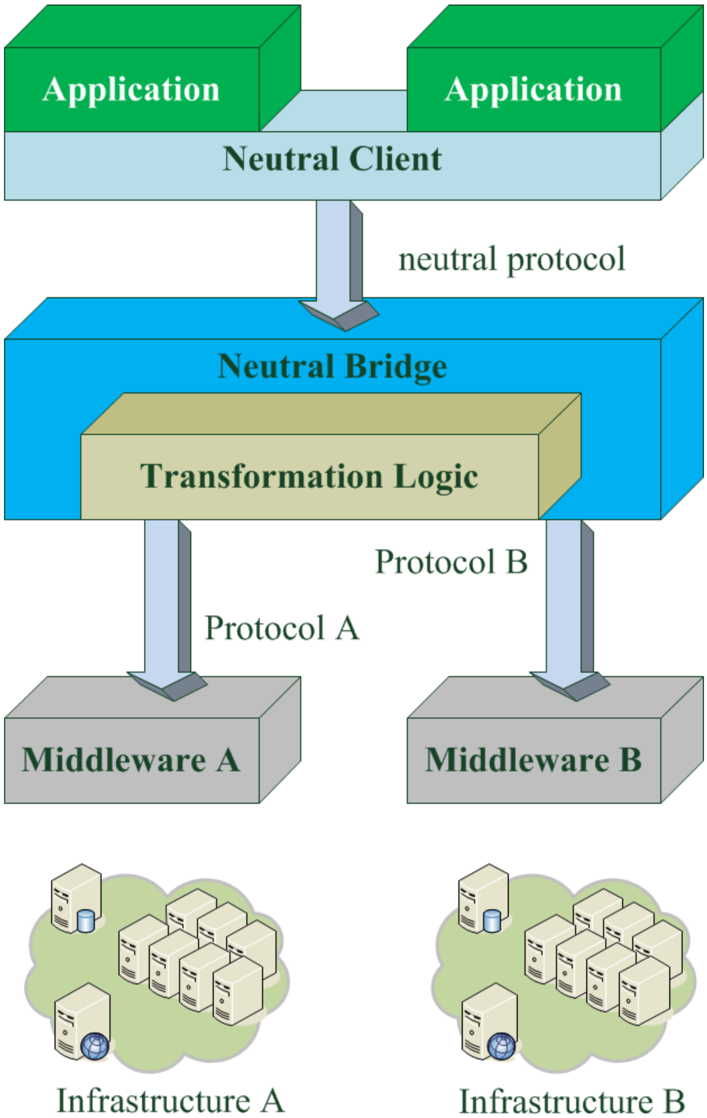

Figure 3: Neutral Bridge Approach

Gateway

As Figure 4 shows, the gateway approach refers to one central entity that is able to translate middleware protocols into other middleware protocols using. It is used, for instance, to realize the interoperability between EGI the CNGrid infrastructure of China.

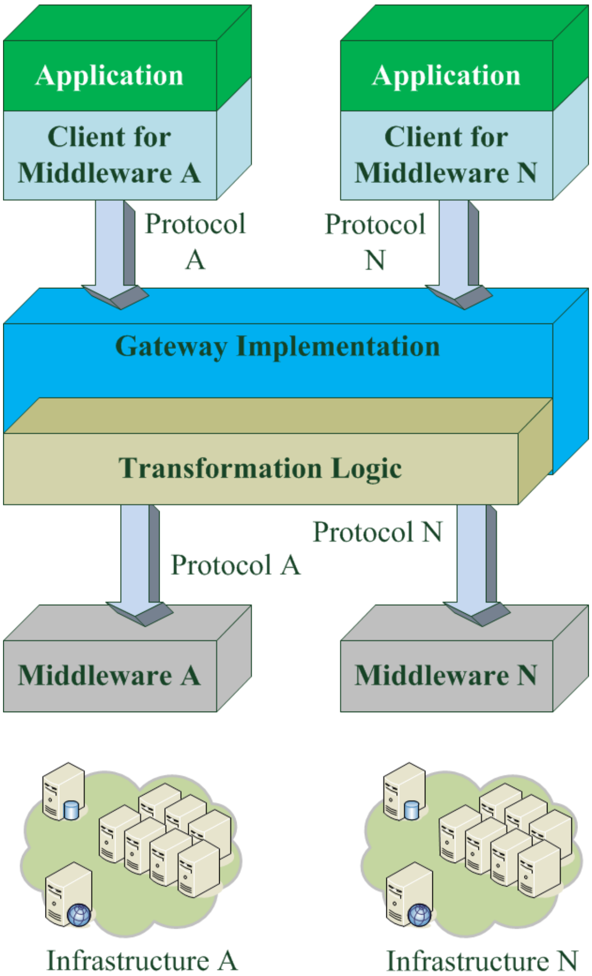

Figure 4: Gateway Approach

Mediator

A mediator (see Figure 5) is similiar to a neutral bridge but instead of using a neutral protocol the respective client technology sticks to one specific protocol and is thus one specialization of the Gateway approach. This approach is adopted in the technologies that make EGI interoperable with BOINC-based infrastructures.

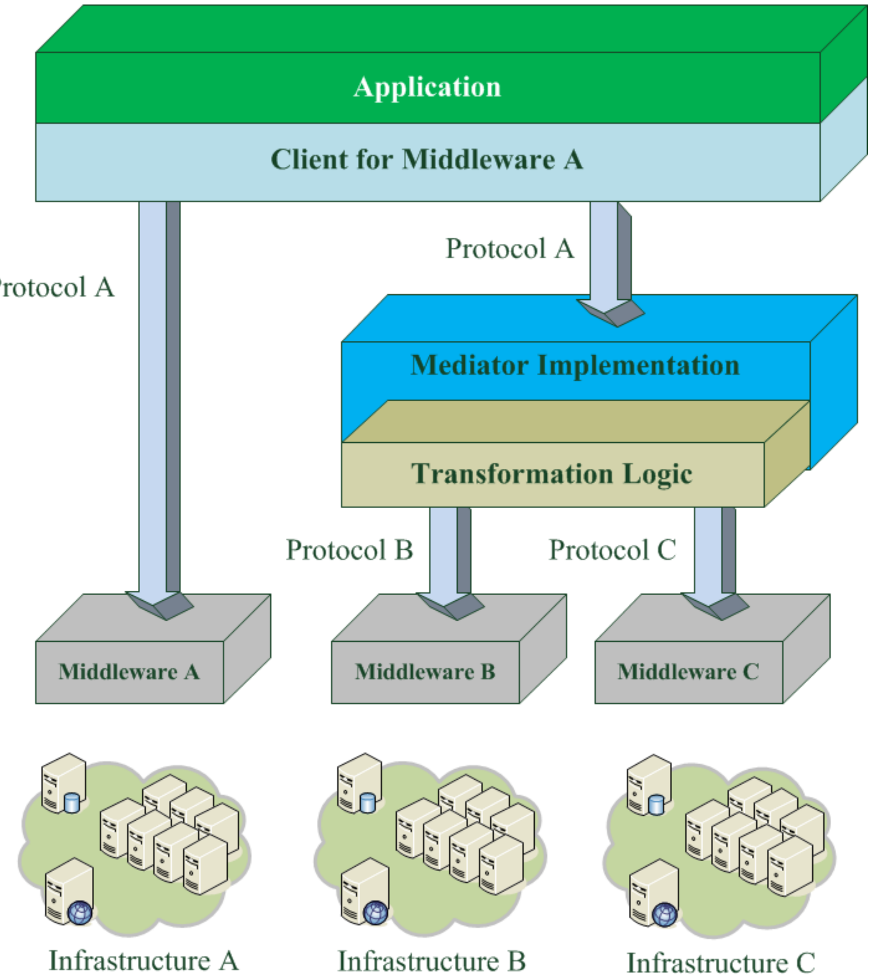

Figure 5: Mediator Approach

Adapter

Adapters (see Figure 6) work like this: A typical Grid middleware client submits with Protocol A a job to the respective Grid middleware which in turn, after processing the job description, executes the job or forwards it to a dedicated adapter. The adapter provides the necessary transformation logic that transforms the job into the format required by the corresponding other Grid middleware. Hence, the difference to other approaches is that the Grid job is actually processed in one middleware stack before being forwarded to another middleware stack B for execution. This approach is adopted to achieve the interoperability between Unicore and gLite.

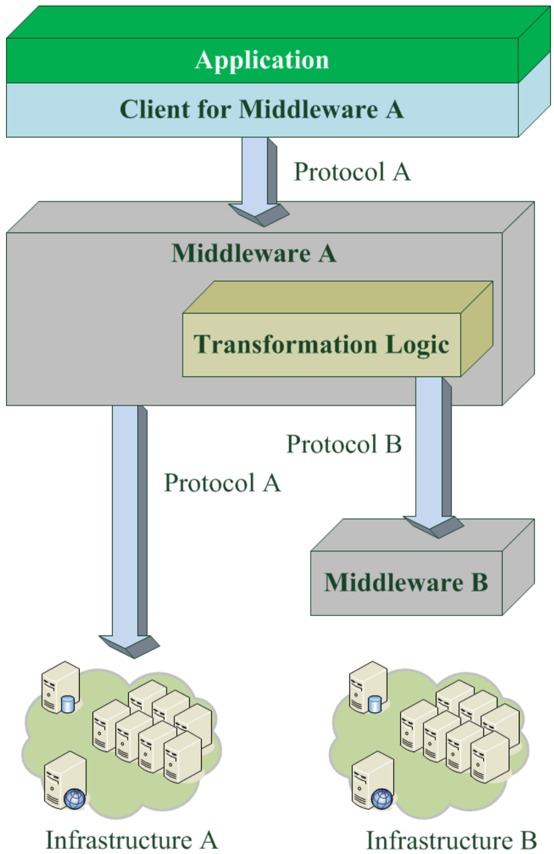

Figure 6: Adapter Approach

Open Standards

The best, but unfortunately also most ambitious, approach to interoperability is to use common open standards (see Figure 7). In the past years, many standardization bodies such as the Open Grid Forum (OGF) have worked on open standards, but we only see a limited number of them deployed on production e-infrastructures. The approach is similiar to the neutral bridge approach, but instead of using a neutral protocol, it uses open standards adopted in the Grid middlewares itself. Please note that this approach does not require any transformation logic.

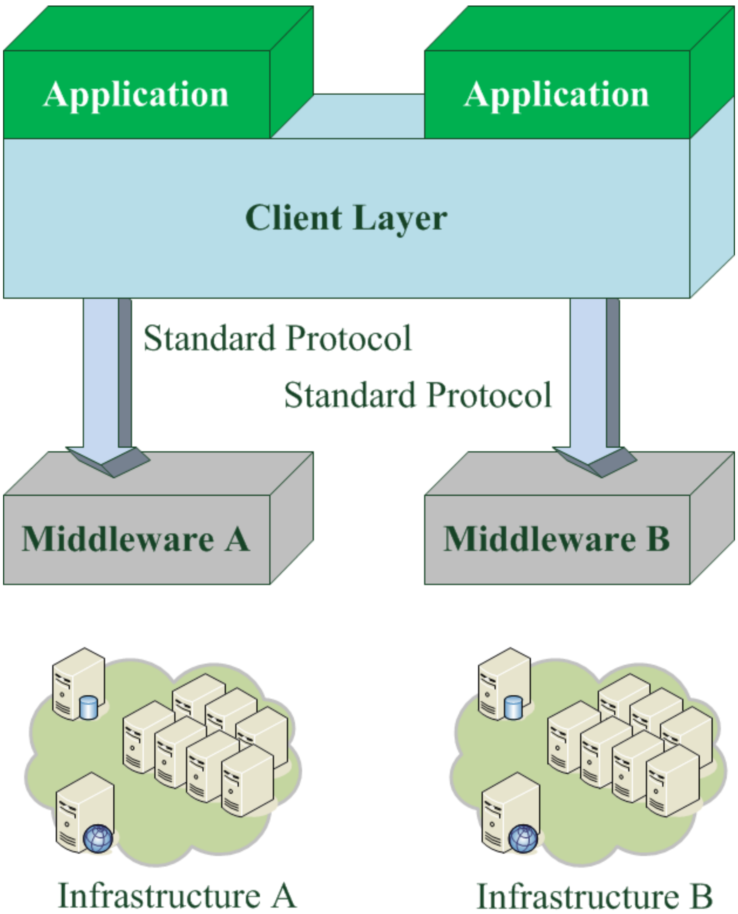

Figure 7: Open Standards Approach

6 Putting It All Together: Future Integration Plan

Given the sustainability aspects (section 3), the identified gaps (section 4) and the various observable interoperability patterns (section 5), we are now able to derive a future integration plan for technical elements that should be taken into account when designing interoperable and integrated trans-continental infrastructures. We briefly describe the starting point of the plan and derive a rough roadmap for the plan to be implemented.

6.1 Starting Point

Currently singular activities in various EU/NSF funded projects propose e-infrastructures to the broader HMR or Earth Science community. Examples are DRIHM, SCIHM [1], VERCE[3], and others. There are already some standardization activities on various levels ongoing (application level, infrastructure level, service levels). As these standardization activities are beyond the scope of this deliverable, we will not comment on the standardization bodies' strategies.

Related to HMR e-infrastructures, several research questions have been addressed and solved individually. Examples are:

- Getting secure and transparent access to computing resources and storage resources through various interoperability patterns (see section 5)
- Getting secure and transparent access to HMR data (DRIHM)
- Designing and executing HMR scientific workflows with chained multi-physics models [5]
- Chaining model executions with or without feedback loops (DRIHM, the EU-funded MAPPER project[4], OpenMI)
- Scheduling the execution of model chains on best suited resources (DRIHM)

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[3] http://www.verce.eu/

[4] http://www.mapper-project.eu

- Seamlessly integrating HPC and HTC resources (EGI, PRACE, XSEDE)
- Passing data between models through standardised interfaces adhering to the geo-temporal type of data (NetCDF-CF, GRIB2, WaterML2, OpenMI)
- Standardized application interfaces (OGF)

A more complete list of scientific data/model/API standards currently being used is given in the following table:

Standard or Technology	Category	Remark
netCDF-CF	Environmental data	Relevant for observational and modelling gridded data as well as for data exchange among model instances
CF (Climate & Forecasting) conventions	Environmental data	Relevant for observational and modelling gridded data as well as for data exchange among model instances
WaterML	Environmental data	Relevant for observational and modelling data point and timeseries
GEOWOW APIs	Environmental data	Relevant for access input data for HMR workflows
ISO19139	Numerical models	Metadata standard for new model engines when added to HMR workflows
OpenMI	Programming API	Relevant for run time data exchange between models, databases and tools in HMR workflows
Grib2	Environmental data	Relevant for observational and modelling gridded data as well as

Standard or Technology	Category	Remark
		for data exchange among model instances
Web Map Service (WMS) interface standard	Environmental data/numerical models	Relevant for requesting geo-registered map images from one or more distributed geospatial databases to be used in HMR workflows
Web Coverage Service (WCS) interface standard	Environmental data/numerical models	Relevant for requesting coverage data in forms that are useful for client-side rendering, and/or as input into HMR workflows

6.2 Objectives

The plan we outline in the following paragraphs aims at defining the key steps necessary for providing a "unified" HMR e-infrastructure in the long run. The roadmap is adapted from similar efforts (like DRIHMS [7], EGI, e-IRG, and others).

While the starting point for the roadmap was described in the previous subsection (based on an analysis we conducted for [2, 4, 5]), the macro objective of the roadmap (establish a "unified" HMR e-infrastructure) is intended to be achieved in a stepwise manner involving several, sometimes transversal, goals. For example, solving the access issues to data and models for HMR applications, migrating simulations to Grids and facilitating the access for everyday Grid users to data, are all mandatory to reach the overall objective despite of the various interoperability patterns.

The plan is arranged along some key categories, specifying their expected achievements and the time period (short-term, mid-term, long-term). In addition, we point out some means (or

key objectives) the fundamental importance of which for HMR communities have been identified. For each time period, we also summarize (some of) the corresponding expected achievements of the community.

6.2.1 Short-Term Objectives

One of the major objectives to be addressed short-term is HMR worldwide community building. Without demand any effort in building e-infrastructures is worthless. To achieve this objective, several activities have been started or are being started. Examples are the work performed by DRIHM, SCIHM and others or the activities defined in the respective Grid, Cloud[5], data, and the HMR scientific consortia.

As community building has a strong governance component, for an e-infrastructure devoted to HMR to achieve efficiency of scale, many organizations need to participate (by granting access to models, data, workflows or by installing resource nodes, access middleware, tools, datasets, etc.). Without legislation and community specific directives this will probably not happen. For this reason we urge the key actors on the political and funding levels to engage in a lasting dialogue aimed at addressing the key issues raised by this roadmap. In close relationship to community building activities, specialized HMR training programs are needed with a focus on specific issues of model coupling and workflow execution on worldwide resources.

Apart from building new or extending existing communities, HMR communities require technical and operational benefits from standardization. This includes (but is not limited to) single sign-on authentication, policy-based authorization of accessing restricted data (support for user roles, directory services, etc.), standardized approaches to access metadata. (see previous sections). A promising example is the RADICAL Cybertools project.[6]

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[5] See for example the EGI Federated Cloud initiative, https://www.egi.eu/infrastructure/cloud/

[6] http://radical-cybertools.github.io/

For a successful deployment of HMR services at large, the identification and discovery of data and resources across communities is needed. Short-term goals are thus standardized ways to not only describe, address and discover data and resources, but also to describe, address and discover HMR related competence centers and Solution Providers.

It should be noted that in parallel to this top-down approach, a demand-driven bottom-up approach is necessary as well. Demonstrations of any kind (videos, live demonstrations, booths at fairs, etc) can create interest and momentum for further adoption of HMR e-infrastructures which in turn may result in an elevated interest at other levels. Thus, this intertwined demand generation for a standardized HMR e-infrastructure needs to be backed in the short- to medium-term by a number of initiatives and the development of respective components on both the Grid- and the HMR-side, by the creation of demonstrators, and by claiming compliance to a standards based profile as proposed in deliverable [6].

The following table outlines (some of) the short-term objectives.

Short-term objectives	to be achieved within the next 1-2 years
Expected Achievements	• expand the HMR –einfrastructure community in terms of number of organisations, number of projects, number of applications worldwide • reduce the technological gaps by providing a set of formal use cases, a set of data and metadata descriptions, and a set of basic workflows services • "gridify" HMR applications to use standards (initially for dissemination purposes, but gradually moving to production-type applications) • Provide wrappers, bridges, and adapters to solve the most urgent interoperability related issues
Means (examples)	• creation of synergies between various HMR and HMR-related communities and continuous promotion and dissemination activities (e.g., the EGU/AGU assembly conferences) • definition and adaptation of an extensibility concept for the DRIHM portal which includes the integration of US requirements and and an XSEDE plug-in • source additional funding

6.2.2 Mid-Term Objectives

The main concern of the mid-term period is overcoming the blocking factors for HMR e-infrastructures, porting of additional models from different disciplines, and facilitating the access for everyday users to HMR data and workflows.

Another issue that needs thorough mid-term investigation is the handling of data within HMR applications. Aspects that need to be examined are data retrieval, access to storage at near real-time and urgent data transfer. Especially the latter is important as on the one hand there is the necessity to transfer huge amounts of data and on the other hand there is a great variety of data formats and access protocols that need to be considered.

The following table outlines (some of) the mid-term objectives.

Mid-term objectives	to be achieved within the next 2-3 years

Expected Achievements	• Identification of and solutions to blocking factors for using HMR e-infrastructures, including
	  ○ data access
	  ○ quality of service
	• Porting of HMR applications (also from different research disciplines)
	  ○ to use identified standards
	  ○ publication of scientific results which could not have been achieved without such a standardized infrastructure
	• Facilitate easy access for citizen scientists to HMR data and workflows
	• Develop a more abstract wrapper, bridge, adaperr concept than short-term

Means (examples)	• increase the number of HMR applications to use standardized services and interfaces and let them benefit immediately for having access to sensors, data, archives, etc. • expose and publish the interfaces and standards • install the basic HMR profile • development of an HMR e-infrastructure aiming at supporting all interoperability patterns (see above) • definition of an enhanced version of the API for data access, integrated single-sign-on, definition of (or contribution to)

Mid-term objectives	to be achieved within the next 2-3 years
	metadata ontologies • define dynamic authentication and authorization policies for accessing data and workflows to assure science related quality-of-service levels on demand • define methods for easy installation of forecasting chains and their visualization

6.2.3 Long-Term Objectives

The long-term objectives are fundamental for a real exploitation of HMR e-infrastructures. However, due to the time range involved, they are hard to predict. Thus, we can only guess and recommend. In any case, they cannot be achieved as long as critical short- and mid-term objectives are still open. Some of the main long-term objectives are outlined in the table below. The effort required for achieving these objectives is more about end user engagement than it is about the deployment of any particular technology.

It should be kept in mind, however, that the development of a standard-compliant middleware and its successful deployment is a cumbersome task. Thus, special emphasis should be given to the ease of adoption, the ease of use, the hiding of complexity from the user, and the support of more complex scientific workflows.

Long-term objectives	to be achieved within the next 4-6 years
Expected Achievements	• Establish a standardized HMR e-infrastructure fully integrating all relevant standards and compliant with the profile(s) defined mid-term ○ The e-infrastructure should facilitate an easy and seamless access to distributed and diverse data and workflows.
Means (examples)	• definition of an interoperability-driven HMR e-infrastructure • make HMR data and workflows readily available via respective infrastructure services • establish within the next 6-8 years a framework to provide timely data of interoperable forecasts for local, national, regional, and international policy makers ○ This requires a capacity building strategy for HMR that will significantly strengthen the capability of all countries to solve HMR related challenges.

7 Conclusion

In this document we outlined a rough future integration plan to establish a "unified" HMR e-infrastructure with technical elements that should be taken into account in future designs of interoperable and integrated trans-continental infrastructures. The plan was based on three ingredients: the DRIHM2US sustainability plan, the gaps identified in [5] and a set of interoperability patterns as they exhibit in e-infrastructures in general and in HMR Grid environments in particular. The plan should be considered supplementary to the sustainability plan exhibited in [6].

8 Acronyms and References

8.1 Acronyms and Abbreviations

Acronym / Abbreviation	Definition
API	Application Programming Interface
BOINC	Berkeley Open Infrastructure for Network Computing
DRIHM	Distributed Research Infrastructure for Hydro-Meteorology
DRIHM2US	Distributed Research Infrastructure for Hydro-Meteorology to United State of America
DRIHMS	Distributed Research Infrastructure for Hydro-Meteorology Study
EGI	European Grid Infrastructure
GUI	Graphical User Interface
HMR	Hydro-Meteorological Research
HPC	High Performance Computing
HTC	High Throughput Computing
ICT	Information and Communications Technology
MoU	Memorandum of Understanding
NGI	National Grid Initiative
OGF	Open Grid Forum

Acronym / Abbreviation	Definition
PRACE	Partnership for Advanced Computing in Europe
SLA	Service Level Agreement
VO	Virtual Organization
WP	Work Package
XSEDE	Extreme Science and Engineering Discovery Environment

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