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Data interoperability requirements of applications

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Glossary

CGI	Coarse-Grained Interoperability
CNRS	Centre National de la Recherche Scientific (French National Centre for Scientific Research)
DCI	Distributed Computing Infrastructure
EGI	European Grid Infrastructure
EMI	European Middleware Initiative
FGI	Fine-Grained Interoperability
jSAGA	Java implementation of the SAGA API
SAGA	Simple API for Grid Applications
SCI-BUS	Scientific gateways-Based User Support project
SSP	SHIWA Simulation Platform
SZTAKI	Magyar Tudomanyos Akademia Szamitastechnikai Kutato Intezete
UoW	University of Westminster
VO	Virtual Observatory
WP	Work Package

Table 1. Glossary

1 Data interoperability

Data Interoperability is a broad area arising from the need of widespread user communities to share and reuse data acquired and stored in different places. Regular use of eScience platforms to speed-up discovery increases the need for data interoperability at a large-scale. Ensuring data interoperability among different users implies **publishing data** (making it known and accessible), giving **means of interpretation** (documenting data so that it can be reused by different actors), and enabling **data transfers** across different resources. This high-level definition of data interoperability covers many different challenges (e.g. the use of interpretable data formats, standard data access protocol, possibly data access control…), some of which are addressed in this document more specifically focussed on ER-Flow objectives.

The SHIWA project[1] has set up a management environment aiming at making multiple workflow systems interoperable. It operationalized its concept through the SHIWA Repository[2], which enables executable workflows sharing, and the SHIWA Simulation Platform[3] (SSP), which enables multi-workflows execution over multiple Distributed Computing Infrastructures (DCIs). However, SHIWA put little emphasis on data interoperability issues. In particular, there is no data repository, no common data specification interface nor means to transfer data across different DCIs within the SSP. As a result, exchanging data across workflow systems or underlying infrastructures remains difficult, and data interoperability is currently implemented manually by end-users inside their workflows. However, cluttering workflows with side concerns such as data transfers activities is cumbersome for end users and it lowers the reusability of workflows uploaded in the SHIWA Repository. The aim of ER-Flow Work Package 4 is therefore to analyze requirements of the supported research communities in scientific data interoperability and their technical implications. This data interoperability study is split in two documents: this document (MS5.1) focuses on user-level requirements, while MS3.1 focuses on technical implications of data interoperability and its impact on the SSP.

1.1 ER-Flow user communities and workflow systems usage

The ER-Flow project involves four pilot user communities: Computational Chemistry, Life Sciences, Astronomy & Astrophysics, and Heliophysics. In addition, it aims at servicing other user communities making use of distributed computing workflow systems, in particular through collaboration with the EGI.eu organization. The pilot user communities already have experience with some workflow systems, in particular:

- WS-PGRADE and UNICORE workflow engine in Computational Chemistry.
- WS-PGRADE and MOTEUR in Life Sciences. The use of Taverna is also being considered.
- WS-PGRADE in Astronomy & Astrophysics. The use of UNICORE workflow engine for access to HPC resources is considered.
- Taverna in Heliophysics.

So the most stringent need relates to WS-PGRADE, UNICORE workflow engine, Taverna and MOTEUR. Many other workflow engines are supported by the SSP platform (*e.g.* Triana, Askalon, Pegasus…), which could be of interest for other communities as well. Integrating the UNICORE workflow engine is in the ER-Flow roadmap.

1.2 Area of study

Scientific workflow systems consume and produce data sets composed of parameters (primitive type values) and raw data (usually stored into files). Each workflow system

[1] SHIWA project: http://www.shiwa-workflow.eu
[2] SHIWA repository: http://repo.shiwa-workflow.eu/
[3] SHIWA Simulation Platform: http://ssp.shiwa-workflow.eu/

manipulates primitive data types using its system-specific representation. The use of array data structures is common among scientific workflow systems, which aim at processing large amounts of scientific data, but the representation of arrays of values is system-dependent.
Workflow systems usually do not consider the content nor the format of raw data stored in files, which are manipulated as opaque entities. In particular, it is the case for all workflow systems considered in ER-Flow. Workflow systems need to get access to these files though, and each system depends on different file symbolic naming schemes that are most often inherited from the underlying Distributed Computing Infrastructure on which the system operates. In some cases, data may be stored in community-specific databases and accessible through domain-specific queries. Most workflow systems are not aware of these databases structures and their query interface though. Data queries are not exposed to the workflow systems: they happen either before workflow execution (to assemble input data sets) or as part of some of the workflow activities, in user business-code. It is the case for all workflow systems considered on ER-Flow and the access to parameters stored in domain-specific databases will not be considered in this study.
Data interoperability issues arise from the need to exchange data between:

- Different workflow activities.
- Different workflow management systems.
- Different distributed computing infrastructures, as different workflow systems may operate on different infrastructures.

The problem of data exchanges between interlinked workflow activities is considered too application-dependent and should be handled by workflow designer. Hence, discrepancies between data representations and file formats manipulated by domain-specific business codes are not addressed in this study.
Conversely, data sets may be exchanged between different workflow management systems in two scenarios at least. Firstly, data sets may be used as intermediate data objects, resulting from a (workflow-based) pre-computation and aimed at being post processed by a different workflow. Secondly, in the SSP multiple workflows may be combined in a meta-workflow as the system enabled coarse-grained workflow interoperability, as illustrated in Figure 1. In this case, data sets are exchanged between different workflow systems as illustrated by orange arrows in Figure 2. In both scenarios, an in-file (serialized) representation of data sets that may be shared between different management systems is needed, as well as mechanisms to map this file representation to workflow invocation parameters. The details of workflow data sets exchanges are discussed in MS3.1.

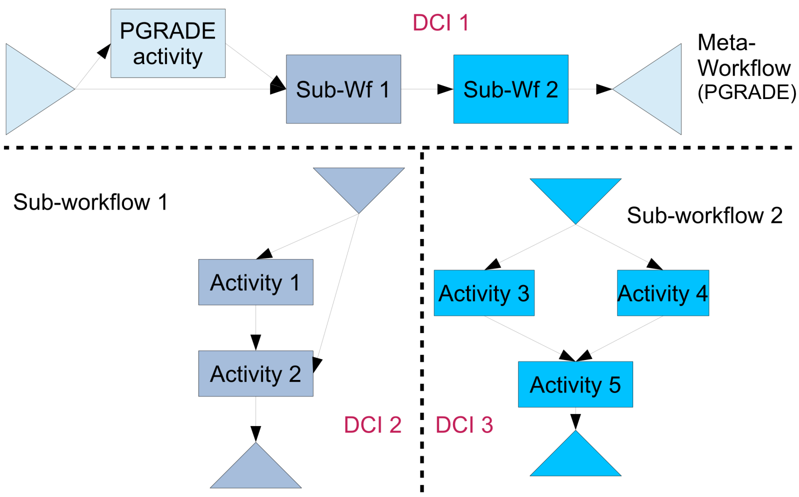

Figure 1. A typical meta-workflow as executed in the SSP: a master PGRADE workflow, executing on computing infrastructure DCI1, embeds a native activity and two sub-workflows as sub-activities. A potentially different workflow engine, potentially using a different computing

infrastructure (DCI2 or DCI3), executes each sub-workflow. The inputs and outputs of the sub-workflows are chained with the master workflow process. The master workflow input and outputs are stored in files and received from / returned to the SSP user interface.

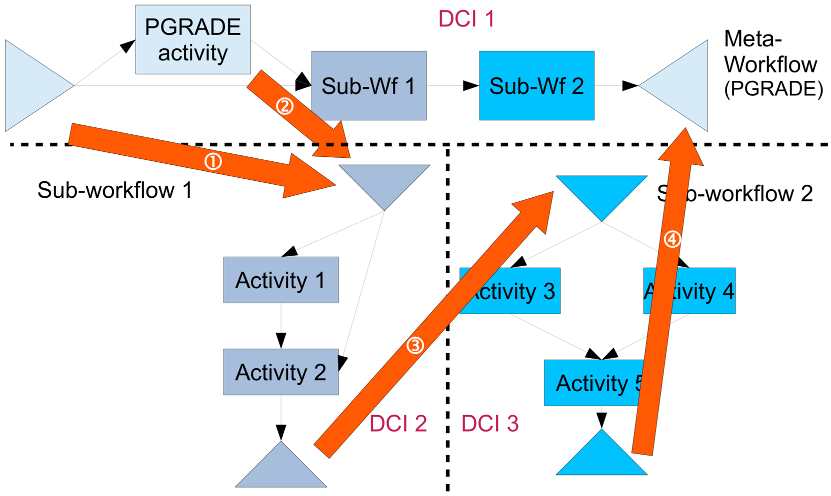

Figure 2. Data transfer needed between the master workflow and the embedded sub-workflows. Sub-workflow 1 receives as input a mixture of data from the master workflow input ① and data produced by the native PGRADE activity ②. Sub-workflow 2 receives as input data produced by sub-workflow 1 ③. Master workflow receives as output data produced by sub-workflow 2 ④.

The need to exchange data sets across different computing infrastructures arises from the dependency of each workflow system to a specific (or a couple of) Distributed Computing Infrastructure(s). The mean of data exchange between different infrastructures is through files and the in-file representation of data sets is also needed for tackling this particular aspect.

The exchange of data sets across different workflow management systems and their underlying computing infrastructure therefore involves:

1. Alignment of workflow system-specific **data representations** (primitive data types, data sets specification and encodings), including an in-file representation.
2. Access to different **file catalogues and file access services** (different symbolic file naming schemes and different data transfer protocols).

The current SSP platform does not manage workflow data sets representation. It only enables the passing of a single file for each master workflow input and output port, and for each sub-workflow input and output. It does not deal with the different sub-systems I/O representation discrepancies, letting to the workflow designer the task of transforming data when needed. It does not recognize non-files parameters nor the structure of data sets. It does not deliver a cross-infrastructures file transfer service either. The remainder of this document outlines the user community requirements for data interoperability.

2 User requirements for data interoperability

2.1 Domain-specific data-interoperability needs

Each scientific domain is making use of its specific scientific data representation format. Some formats become widely accepted and facilitate the exchange of data between different domain applications. In ER-Flow for instance:

- Computational Chemistry uses the XYZ format coordinates[4] and the Protein Data Bank (PDB) format[5] to three-dimensional structure of molecules.
- Life Sciences uses different image formats, among which DICOM[6], as well as several various radiology metadata formats.
- Astronomy & Astrophysics adopted the Flexible Image Transport System (FITS) format[7] for representing astronomical observations.

All the formats cited above aim at exchanging data between domain business applications sharing the same file format. File format converters are used for dealing with different data representation formats. Scientific workflow systems manipulate data files in a domain-agnostic manner, without consideration of the actual content, format, nor coherency of these files. Data files representation are managed in workflows implicitly through format-aware scientific data processing codes or explicitly, through format conversion activities. In both cases, it is up to the workflow designer to consider file format support by each workflow activities. This information is considered too domain-specific and not accessible from the workflow management system. While files formats are not handled in workflow systems, file names are manipulated through their symbolic file identifiers though.

Beyond domain-specific data formats, scientific workflow systems often manipulate primitive data type parameters such as numbers, character strings or file symbolic reference names. Conversely to domain-specific file formats, these primitive types are shared by all workflow systems and they may be exchanged as part of the workflow input and output data sets. Concrete recommendations for encoding of primitive data types using the W3C XSD standard[8] are discussed in MS3.1. Only the boolean, long, double, string, anyURI (for file identifiers) and base64Binary (for binary data) data types are considered in scientific workflow systems. In addition, XSD complex type definition mechanisms are considered for defining homogeneous arrays of primitive data types or multi-level homogeneous arrays in order to represent complete scientific data sets. The advantages of using XSD are its standard data representation and standard file serialization in XML. Other, non-primitive-data is stored and manipulated as binary data in files. Distributed files are identified by symbolic name identifiers can be represented in XSD data sets as URIs.

There are therefore no strong requirements expressed by ER-Flow user communities for domain-specific interoperability needs. The data interoperability requirements arise from

1. The need to exchange parameters in the form of primitive data types; and
2. The current limitations of the SSP to exchange data sets over different workflow management systems.

MS3.1 gives more details on the insights on parameters representation and cross-DCI file transfers. It also addresses the practical problem of mapping the standardised parameters representation on the specific invocation interface of each workflow management system integrated in the SSP.

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[4] XYZ coordinates format, http://en.wikipedia.org/wiki/XYZ_file_format
[5] Protein Data Bank format (PDB) http://en.wikipedia.org/wiki/Protein_Data_Bank_(file_format), http://www.wwpdb.org/documentation/format33/v3.3.html
[6] Digital Image and Communication in Medicine (DICOM), http://en.wikipedia.org/wiki/DICOM, http://dicom.nema.org
[7] Flexible Image Transport System (FITS), http://en.wikipedia.org/wiki/FITS, http://fits.gsfc.nasa.gov/
[8] World Wide Web Consortium XML Schema Definition (XSD), http://www.w3.org/TR/xmlschema11-1/

2.2 File symbolic referencing and catalogues

While files formats are not handled in workflow systems, the file themselves are manipulated through their logical identifiers. In Distributed Computing Infrastructures, scientific data files are stored on possibly heterogeneous storage resources and referenced to through an infrastructure-specific symbolic file name mechanism. File catalogues are used to structure file sets. Existing file catalogues range from simple file system-like file hierarchy views over stored files, to complex databases including file references and rich associated metadata that enable advanced search over file data sets.

The Astronomy community probably has the more elaborated distributed file catalogues. The Virtual Observatory[9] (VO) is an international-scale effort to publicly share astronomy data. It hosts a registry of regional astronomy data registries over which it provides a homogeneous view and data location services. It standardizes data access and data transfer across catalogues. The catalogues are based on relational databases through which advanced data search facilities are provided. Data sets are finally identified through lists of URLs that enable direct access to files through HTTP. In the context of EGI-InsPIRE project Work Package 6, an effort is in progress to create a bridge between the VO catalogues and applications (including workflows). However, this is still a work in progress.

Through the Molecular Simulation Grid portal[10] (MoSGrid), the Computational Chemistry community similarly accesses a single database covering the 3 sub-domains covered (quantum physics, molecular dynamics and molecular docking). The MoSGrid database indexes files stored in the UNICORE Extreme FS file system. Files compliant to the Molecular Simulation Markup Language (MSML) provide rich information sets used to populate the MoSGrid relational database.

Finally, the Life Sciences community mostly make use of the LFC file catalogue[11] maintained as part of the European Middleware Initiative (EMI). LFC is a relational catalogue mapping logical file names (URIs) to physical replicas of data files. It has a limited capability for storing user-defined metadata associated to each logical file. It provides a hierarchical view of files stored in virtual folders. Some specific catalogues may also be in use, such as the XNAT data management system[12] used in neuroradiology. A WS-PGRADE wrapper portlet has been implemented for XNAT. It enables input data pre-staging and output data post-staging in the XNAT catalogue.

The specific catalogues in use within each user communities are currently considered too domain-specific for workflow management level, although some initiatives show a growing interest for repository-aware workflow management systems (VO catalogue bridge and XNAT wrapper for WS-PGRADE for instance). All computing infrastructures underlying the workflow systems supported by ER-Flow currently use URIs to reference files. URIs are rich identifiers which usually contain target file server identification, file access protocol and server-specific file identification name. These URIs ensure the uniqueness of file names across distributed resources and facilitate their retrieval.

Ensuring file data sets interoperability across multiple workflow systems based on different Distributed Computing Infrastructures usually requires copying files across the different infrastructure data management systems and replacing file symbolic identifiers. File transfers across DCIs is a notoriously difficult problem due to the different file access / transfer protocols in use and the need for a common authentication & authorization framework among the target DCIs [Korkhov 11]. Several tools tackles this issue though, such as the jSAGA library[13] or the SCI-BUS Data Bridge service[14] introduced in MS3.1. A secondary concern is the limitation of the current coarse-grained interoperability mechanism

[9] Virtual Observatory (VO), http://www.ivoa.net
[10] Molecular Simulation Grid (MoSGrid), https://mosgrid.de
[11] LCG File Catalogue (LFC), http://www.eu-emi.eu/products/-/asset_publisher/1gkD/content/lfc-3
[12] Imaging Informatics Software Platform (XNAT), http://xnat.org/
[13] Java Simple API for Grid Applications (jSAGA), http://grid.in2p3.fr/jsaga/
[14] Scientific Gateway-Based User Suport (SCI-BUS), https://www.sci-bus.eu

implemented in the SSP (with WS-PGRADE master workflow engine), which only supports single file exchange for each sub-workflow I/O. The use of a file archive format, such as the ORE format[15], is recommended to bundle several files when needed.

2.3 Semantic data

Data semantic description is considered as a key towards data interoperability nowadays. Data semantic technology arose from the emergence of the *Semantic Web*[16] and the need to ease data interlinking and interpretation. In this context the *World Wide Web Consortium* (W3C) defined multiple standards to explicit the semantics of data, including vocabulary definition languages (e.g. RDFS[17] and OWL[18]) and semantic annotation formats (e.g. RDF[19]). The formal definition of data semantics through a vocabulary facilitates the alignment of heterogeneous data sources onto a shared reference. It thus primary addresses the challenge of data interoperability at the level of data representations. In addition, eScience platforms increasingly use semantic description resources to link the semantics of computations (as contained in workflow programs) and the semantics of data, *e.g.* through the production of provenance traces upon data generation. Semantic information therefore becomes a vector to facilitate data reuse and data generation reproducibility.

Among the pilot scientific communities involved in ER-Flow, there is only a limited use of semantic technologies so far. Metadata may be extensively used to describe and make data searchable, *e.g.* in the Virtual Observatory catalogues, but there are no widely accepted reference semantic vocabulary, neither in Astronomy nor in Computation Chemistry where pivot format files (PDB, FITS) are widely adopted as data sharing means. In Life Sciences though, and most particularly in medicine and in radiology, many ontologies have been developed. Some *de facto* standards emerged such as the XNAT data model or the Foundational Model of Anatomy[20] (FMA). The use of semantic technology goes beyond data description and is used *e.g.* for data provenance (using OPM[21] or PROV[22] models).

The impact of semantic technologies will be studied in depth in the future of WP4 activity within ER-Flow (Task 4.4).

15 Object Reuse and Exchange (ORE) format, http://www.openarchives.org/ore/
16 Semantic Web, http://www.w3.org/standards/semanticweb/
17 RDF Vocabulary Description Language (RDFS), http://www.w3.org/TR/rdf-schema/
18 Web Ontology Language (OWL), http://www.w3.org/standards/techs/owl
19 Resource Description Framework (RDF), http://www.w3.org/TR/rdf-mt/
20 Foundational Model of Anatomy (FMA), http://sig.biostr.washington.edu/projects/fm/
21 Open Provenance Model (OPM), http://openprovenance.org
22 PROV specification for provenance on the Web, http://www.w3.org/TR/prov-primer/

3 Conclusions

There are no outstanding requirements expressed by ER-Flow user communities for domain-specific data interoperability needs. The cross-domain analysis reported in this document shows that all pilot communities make use of general-purpose scientific workflow systems. The generic data interoperability requirements arise from:

1. The need to exchange parameters in the form of primitive data types; and
2. The current limitations of the SSP to exchange data sets over different workflow management systems.

Addressing these challenges implies significant changes to the SSP execution platforms as detailed in MS3.1. On the application domains side, in the future the work will focus on making explicit the semantics of scientific workflow data transformation processes and the data thus generated. Beyond the syntactic pivot data format proposed in MS3.1, this work will enable rich description of data sets produced on an eScience platform such as the SSP, including data provenance information and data explication, for better exploitation and better reuse of scientific data.

References

[Korkhov, 11] Korkohv V., Krefting D., Kukla T., Terstyanszky G., Caan M. and Olabarriaga S., “Exploring workflow interoperability tools for neuroimaging data analysis”, Proceedings of the 6th workshop on Workflows in support of large-scale science (WORKS’11), Seattle, USA, November 2011, pp 87-96, ACM. http://dx.doi.org/10.1145/2110497.2110508.

[MS3.1] Montagnat J. and Cerezo N., “Data interoperability requirements of the infrastructure”, MileStone 3.1, ER-Flow project, 2013.