Software Architectures to Integrate Workflow Engines in Science Gateways

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Abstract

We investigate software architectures commonly used to integrate workflow engines in science gateways. Based on our experience with the development and operations of the CBRAIN and VIP science gateways, and our past involvement in the SHIWA project, we abstract software components and interactions in 6 architectures that we use to classify 18 systems. We compare these architectures using metrics measuring global complexity, robustness, extensibility, scalability and other specific features. Results show the pros and cons of the different architectures: tight integration and sub-tasking are the simplest architectures and should therefore be the easiest to implement and the most robust ones, most architectures perform the same in terms of extensibility, the pool model is the most scalable and meta-workflows are only available in nested workflows and workflow import. These results provide insights for software architects on how to integrate science gateways and workflow engines.

Keywords: Workflow engines, science gateways, software architecture.

1. Introduction

Workflow engines are critical components of the ecosystem of tools and services offered by science gateways to leverage distributed infrastructures for the efficient execution of applications through the web. Several software architectures can be adopted to integrate workflow engines in science gateways, with important consequences on the required development effort and on the resulting system. This paper describes, exemplifies and compares such architectures, based on system-independent representations of their main components and interactions.

Our analysis is fed by experience gathered from the development and sustained operation of the CBRAIN [1] and VIP [2] science gateways for medical image analysis during the past 7 years. It also builds on the lessons learned from several science gateway and workflow-related projects, including SHIWA[1] and related initiatives.

The remainder of this Section provides background information and definitions about workflow engines, science gateways and infrastructures. In Section 2, we describe 6 architectures in a consistent framework based on the functional interactions between the main software components involved. In Section 3, we introduce metrics to measure global complexity, robustness, extensibility, scalability and other specific features of the architectures. We use these metrics to evaluate and compare the 6 architectures. The paper closes on a discussion and conclusion that highlight architectural recommendations for science gateway and workflow engine architects.

1.1. Workflow engines

In the last decade, the e-Science community has developed workflow systems to help developers access distributed infrastructures such as clusters, grids, clouds and web services. These efforts resulted in tools such as Askalon [3], Hyperflow [4], MOTEUR [5], Pegasus [6, 7], Swift [8], Taverna [9],

[1] `http://www.shiwa-workflow.eu`

Triana [10], VisTrails [11], WS-PGRADE [12] and others. Such workflow engines usually describe applications in a high-level language that offers specific data and control flow constructs, parallelization operators, visual edition features, links with domain-specific tool repositories, provenance recording, among other features. An overview of workflow systems features and capability is available in [13].

At the same time, toolboxes were emerging in various scientific domains to facilitate the assembly of software components in consistent "pipelines". In neuroimaging, our primary domain of interest, tools such as Nipype (Neuroimaging in Python, Pipelines and Interfaces [14]), PSOM (Pipeline System for Octave and Matlab [15]), SPM (Statistical Parametric Mapping [16]) and FSL (FMRIB Software Library [17]) provide abstractions and functions to handle the data and computing flow between processes implemented in a variety of programming languages. Such tools were interfaced to computing systems, in particular clusters, to handle high-throughput task executions. For instance, FSL can launch tasks on SGE through its fsl_sub tool, Nipype has execution plugins for S/OGE, Torque, IPython, ssh and multi-processor servers, and PSOM is interfaced to Torque, SGE, MOAB, LSF, and HTCondor. Some of these tools also support advanced features such as provenance tracking (Nipype, PSOM), redundancy detection across analyses to avoid re-computation (PSOM), and so on. A wide-array of workflows have been implemented using these pipelines and are now shared across neuroimaging groups world-wide. These domain-specific engines represent a tremendous opportunity for science gateways to leverage existing tools and applications. They nicely complement e-Science engines that are more oriented towards the exploitation of distributed computing infrastructures, in particular grids and clouds.

For the sake of the analysis conducted in this paper, we define a *workflow engine* (also abbreviated *engine*) as a piece of software that submits interdependent computing *tasks* to an *infrastructure* (local server, cluster, grid or cloud) based on a workflow description (a.k.a *workflow*) and using input data that may consist of files, database entries or simple parameter values. Although simplistic, this definition covers both e-Science and domain-specific engines. Some workflow engines, usually e-Science ones, may transfer data across the infrastructure, and others, usually domain-specific ones, may leave this role to external processes. Workflows may be expressed in any language, including high-level XML or JSON dialects such as Scufl or Hyperflow, and low-level scripting languages such as Bash.

1.2. Science gateways

Science gateways are used to share resources in a community and to provide increased performance and capacity through facilitated access to storage and computing power. They are often accessible through a web interface that helps users manage access rights, data transfers, task execution and authentication on multiple computing and storage locations. Workflow engines are part of this ecosystem as core components to implement and execute applications.

Integration between workflow engines and science gateways varies across systems. Some science gateways may be tailored to a particular engine that manages critical functions such as task execution, data transfers and authentication. Other gateways may be more general and host applications executed by different types of engines. Extensibility is an important property of the integration, as new workflows are added frequently, different types and versions of workflow engines may be integrated over time, and different kinds of infrastructure can be targeted.

Scalability is also an important concern, since science gateways are multi-user systems that manage substantial amounts of data and execute computationally-intensive analyses. To this end, science gateways may include different instances of the same engine type and implement some load-balancing policy among them. They may also use advanced task scheduling policies on the infrastructure, e.g. to ensure fairness among users [18, 19] or to improve fault-tolerance [20, 21].

Robustness is a highly desirable characteristic in production gateways. In this respect, the multiplicity of software components and interactions involved in architectures is a challenge as it often leads to complex systems. Architectures showing reduced system complexity will greatly facilitate the implementation effort towards robust interactions which, in turn, have a positive impact on characteristics such as gateway predictability, transparence, general reliability and results traceability and reproducibility; characteristics that are also key to a good user experience.

Specific features may also be available in science gateways, such as data vizualisation and quality control, workflow edition, debugging instruments, social tools among users, etc.

Various science gateways have been developed, including frameworks used as building blocks to assemble science gateways. The main frameworks are Apache Airavata [22], the Catania Science Gateway Framework [23] and WS-PGRADE/gUSE [12]. Numerous science gateway instances were built using such frameworks [24, 25]. Other gateway instances were also built independently from any framework, using regular web development tools and libraries to access distributed systems. CBRAIN and VIP are two such science gateways, from which we gathered experience about the architectures described in this paper.

CBRAIN[2] [1] is an open-source[3], web-based collaborative platform addressing the challenges of data-heavy, computation-intensive neuroimaging research. It offers transparent web-based access to remote data sources, distributed computing sites, and an array of processing and visualization tools, within a secure environment. CBRAIN is deployed at a wide range of computing sites, including a network of national HPC centers in Canada, one in Korea, one in Germany, and on numerous local servers. As February 2016, CBRAIN has served over 420 users across 50 cities in 22 countries and has a national computing allocation of 660 CPU years per annum.

The Virtual Imaging Platform (VIP[4]) [2] is a web portal for medical simulation and image data analysis. It leverages computing and storage resources available in the biomed Virtual Organization of the European Grid Infrastructure (EGI) to offer an open service to academic researchers worldwide. VIP completely masks the infrastructure to enable a transparent user experience. It uses the MOTEUR workflow engine [2] and the DIRAC pilot-job framework [26] to execute applications on EGI. Almost 900 users were registered in VIP by April 2016 and the average CPU consumption between January 2013 and March 2016 was 35 CPU years per month.

The architectures described hereafter also build on experience with the SHIWA Simulation Platform [27]. The SHIWA Simulation Platform is a WS-PGRADE/gUSE science gateway that was developed in the European projects SHIWA[5] and ER-flow[6]. It focuses on workflow interoperability for various disciplines, in particular through the building of meta-workflows, i.e. workflows that are built out of other workflows. It implements the so-called Coarse-Grained Interoperability framework where workflow engines are integrated in the science gateway as other applications and invoked through a dedicated service. The Fine-Grained Interoperability framework was also developed in the SHIWA project, where conversions between workflow languages are achieved through a common intermediate representation [28].

1.3. Infrastructures

In this paper, infrastructure consists of the computing and storage resources involved in the workflow execution, as well as the software services used to access these resources. Infrastructures can be composed of computing or file servers, databases, clusters, grids or clouds. Some workflow engines and science gateways may assume specific characteristics about the infrastructure, such as the presence of a shared file system between the computing nodes, the availability of a global task meta-scheduler, the presence of a file catalog, etc. In the analysis presented below, such specific functions are not discussed. Instead, we consider the infrastructure as an abstract system that can execute tasks and store data regardless of the enabling mechanisms.

2. Architectures

Architectures to integrate workflow engines in science gateways are diagrammed in Figure 2 using the graphical notations shown in Figure 1.

Architectures are described from their main software *components* and *interactions*. Software components include science gateway and infrastructure in all architectures while workflow service, workflow pool and agent are involved in some architectures only. The workflow engine itself is represented by a specific symbol enclosed in a dotted rectangle.

Software interactions among these components are represented with labeled, plain black arrows.

[2] http://cbrain.mcgill.ca
[3] https://github.com/aces/cbrain
[4] http://www.creatis.insa-lyon.fr/vip
[5] http://www.shiwa-workflow.eu
[6] http://www.erflow.eu

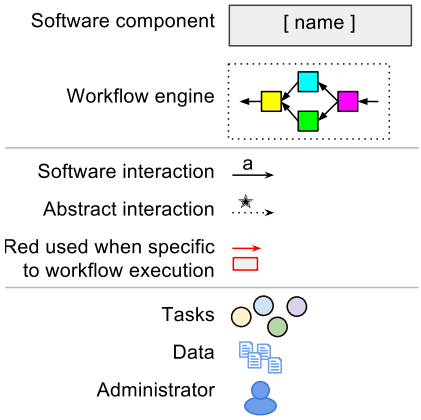


Figure 1: Graphical notations

Abstract interactions are specific types of interactions that may be implemented using different components and interactions. They are represented with dotted arrows and labeled with $*$. An architecture that has an abstract interaction is an abstract architecture that can be instantiated in various ways.

Red color is used to represent the components and interactions that are specific to workflow execution, i.e. that are not involved in any other process. Tasks refer to computing tasks created by the workflow engine and executed on the infrastructure. Data represents any type of file or database involved in workflow execution and stored on the infrastructure. It does not cover workflow parameters such as strings, numbers, etc. Administrator refers to a science gateway user with extended privileges to install applications.

The remainder of this section describes the different types of interactions involved in the architectures. Architectures are then detailed and illustrated using examples of real systems. Table 1 summarizes the classification of a few systems by architecture.

2.1. Interactions

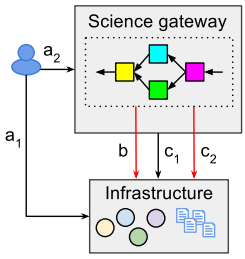
The interactions involved in the architectures are described below and labeled consistently with the notations used on Figure 2.

(a) Workflow integration: consists in adding a new workflow to the system so that users can execute it. It is triggered by an administrator of the science gateway and it results in an interface, for instance a web form, where users can enter the parameters of the workflow to be executed. The interaction has two aspects: (a_1) the programs used in the workflow are installed on the infrastructure, which may require administrative privileges on the infrastructure; (a_2) the workflow is configured in the science gateway so that it becomes available to users. Note that integrating a workflow is not the same process as integrating a workflow *engine*.

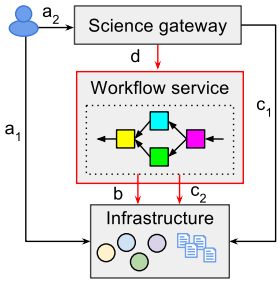
(b) Task control: operations to manage tasks on the infrastructure, including: authentication, submission, monitoring, termination, deletion, etc. Controlling tasks requires to deal with the heterogeneous batch managers and meta-schedulers that might be available on the infrastructure. When the infrastructure is a grid or a cloud, it may for instance be achieved using libraries that implement standards such as SAGA (Simple API for Grid Applications [40]), DRMAA (Distributed Resource Management Application API [41]), or OCCI (Open Cloud Computing Interface [42]).

(c) Data control: operations to manage data on the infrastructure, such as: upload, download, deletion, browsing, replication, caching, etc. Data movements can be triggered by the user in the science gateway (c_1), to upload input data or download processed data. They can also be performed by the workflow engine (c_2), to transfer workflow data (inputs, outputs, or intermediate results) across the infrastructure so that tasks can use it. The infrastructure might offer various data storage backends with heterogeneous interfaces. Marc-eI meant, "using c1", a user in some platforms (CBRAIN), can trigger some operations across the infrastructure, as in c2... not just up/download data. And I clearly see now that this is in fact the case in III, c is not differentiated. Closing this thread for good. Tools and services such as JSAGA [43] or Data Avenue [44] can be used to homogeneize these interfaces.

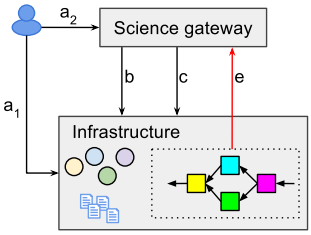
(d) Workflow control: operations to control workflow execution in an engine, including: workflow submission, monitoring, termination, etc. Workflow control can be coarse-grained (black box) or fine-grained (white box). In a coarse-grained model, the various tasks created by a workflow execution are masked and the user only has a global view of the workflow execution. In a fine-grained model, user is exposed to the workflow topology, i.e. to the outputs of the individual tasks, their statuses and so on.



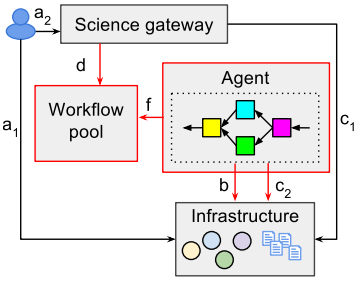
(I) Tight integration



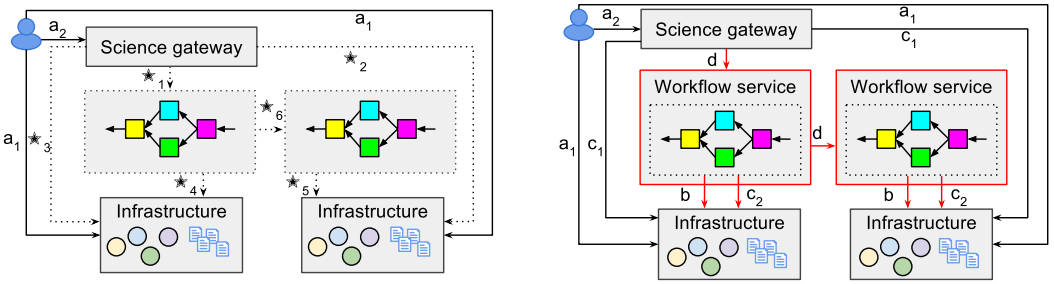
(II) Service invocation



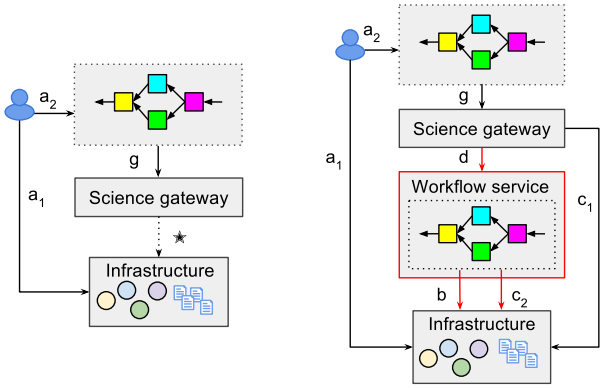
(III) Sub-tasking



(IV) Pool



(V) Nested workflows. Left: abstract model. Right: instantiation with service invocation.



(VI) Workflow import. Left: abstract model. Right: instantiation with service invocation.

Figure 2: Architectures

Architecture	Systems
Tight	Catania Science Gateway Framework [23], Distributed application runtime environment (DARE [29]), DECIDE [25][c,n], LONI Pipeline Environment[n] [30]
Service	Apache Airvata [22], e-BioInfra [31][w,n], HubZero with Pegasus [32], MoSGrid [33][w], System in [34], Vine Toolkit [35], Virtual Imaging Platform [2][n], WS-PGRADE/gUSE framework [12], Science gateways in [24][w]
Sub-task	CBRAIN and PSOM [36][n], CBRAIN and FSL[n]
Pool	SHIWA pool [37]
Nested	SHIWA Simulation Platform (Coarse-Grained Interoperability [27])[w], HubZero with Pegasus (via hierarchical workflows) [7], Tavaxy [38].
Import	SHIWA Simulation Platform (Fine-Grained Interoperability) [28][w], Tavaxy [38], system in [39].

Table 1: Classification of science gateways based on the architecture used to integrate workflow engines. [c]: based on the Catania Science Gateway Framework. [w]: based on WS-PGRADE/gUSE. [n]: used for neuroimaging.

(e) Sub-task control: operations used by tasks to submit sub-tasks on the infrastructure, including: submission, monitoring, termination, deletion, etc. Sub-task control is similar to interaction b, except that information about the parent task, which submitted a sub-task, is usually available and used for additional control. For instance, the parent task may wait for all its sub-tasks to complete before finishing, and conversely all the sub-tasks may be terminated if the parent task is killed.

(f) Pool-agent: specific to the pool architecture described in Section 2.5. This is an interaction used when agents retrieve work from a central pool. It covers agent registration and de-registration to the pool, protocols to send work from the pool to the agent, mechanisms to update work status, and so on. A similar type of interaction is used in pilot-job systems [45] and other agent-based computing models.

(g) Workflow conversion: translation from one workflow language to another one. This interaction may not be available or implementable for every workflow language. It has been developed mostly for well-structured and relatively simple workflow language such as between GWorkflowDL and Scufl [46], and between the 4 languages that were involved in the SHIWA initiative. In SHIWA, workflow conversion is done through an intermediate representation, the Interoperable Workflow Intermediate Representation [47], which allows to convert among n workflow languages using $2n$ interactions instead of n^2.

2.2. Tight integration

See Figure 2(I). The workflow engine is tightly integrated with the science gateway, which means that it is deployed on the same machine and potentially shares code, libraries and other software components with the science gateway. For instance, the workflow engine might be a portlet in a Liferay portal or a controller in a Ruby on Rails application. The workflow engine and the science gateway usually share a database where application, users and other resources are stored. In this model, task and data control are both initiated from the science gateway. Interactions b and c_2 are initiated from the workflow engine while c_1 comes from other parts of the science gateway, for instance a data management interface. As in any other model, the installation of new workflows in the science gateway (a_2) and infrastructure (a_1) is done by an administrator, for security reasons. This is the model adopted in the Catania Science Gateway Framework [23] (see specific documentation on workflows[7]), in the Distributed application runtime environment (DARE [29]), in Galaxy [48], and in LONI Pipeline Environment [30]. Note that tightly integrated architectures may provide advanced workflow edition features which are not covered by our analysis.

2.3. Service invocation

See Figure 2(II). The workflow engine is available externally to the science gateway, in a service. The science gateway controls the service through a specific interaction (d) that might be implemented as a web-service call (e.g., RESTful or SOAP), as a command-line or as any other method that offers a well-defined interface to the workflow engine. The workflow engine might be invoked either as a black box that completely masks the infrastructure and tasks, or as a white box that allows for some interaction with them. The workflow engine is responsible for controlling the tasks on the infrastructure (b) and for performing the required data transfers to

[7] http://bit.ly/1oQrzvQ

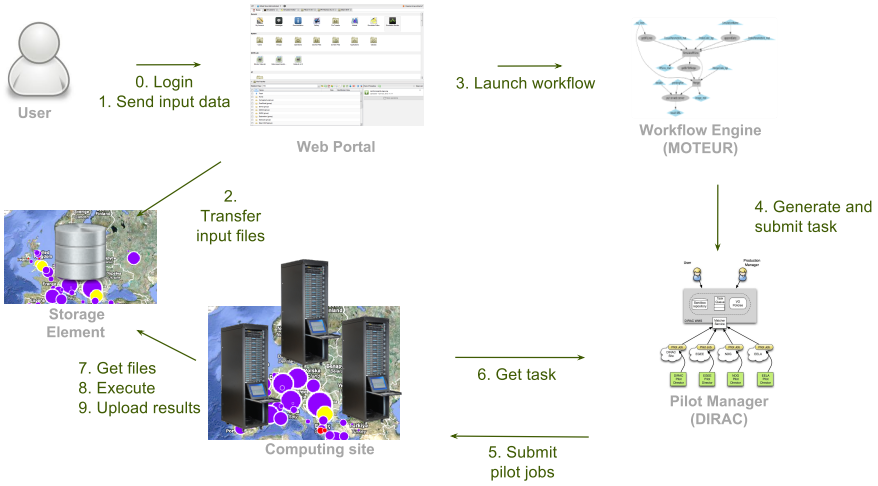


Figure 3: Architecture of the Virtual Imaging Platform (service invocation). Step `3` corresponds to interaction `d` on Figure 2, step `2` corresponds to interaction c_1, and step `4` maps to interactions `b` and c_2 (in VIP, workflow data transfers are performed by the tasks and embedded in their descriptions).

execute them (c_2). User data is usually managed through the science gateway (c_1), although it might as well be delivered by the workflow engine directly to the user.

This architecture is largely adopted, in systems such as Apache Airvata [22], Vine Toolkit [35], Virtual Imaging Platform [2], the system in [34] and the WS-PGRADE/gUSE framework [12]. The integration between the HubZero science gateway and the Pegasus workflow engine performed in [32] also uses a service architecture where the `d` interaction is implemented as a set of calls to Pegasus' command-line tools (e.g., pegasus-status, pegasus-plan, etc.). Figure 3 shows the architecture of the Virtual Imaging Platform, where the MOTEUR workflow engine [5] is invoked through a service.

2.4. Sub-tasking

See Figure 2(III). The workflow engine is a particular task that can submit sub-tasks to the science gateway through interaction `e`. The workflow engine keeps track of the dependencies between the sub-tasks, but their execution is delegated to the science gateway that executes them on the infrastructure through interaction `b`. Although the science gateway has no global vision of the workflow, it can keep track of the sub-tasks submitted by a given task, for instance to be able to cancel them when the task is canceled. The science gateway may also implement mechanisms to facilitate the handling of task dependencies, for instance basic dependency lists as available in most batch managers (see for instance attribute `depend` of option `-W` in Torque[8]).

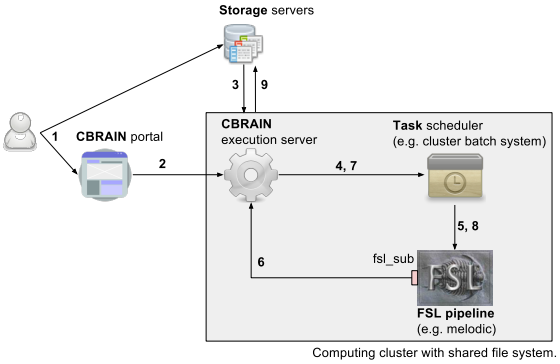
The science gateway also transfers both user and workflow data across the infrastructure, so that interactions c_1 and c_2 are both covered by `c`. In practice, both c_1 and c_2 can be implemented using the same pieces of code.

The sub-tasking architecture is implemented in CBRAIN [1] where it is used to integrate the FSL toolkit [17] and the PSOM workflow engine [15].

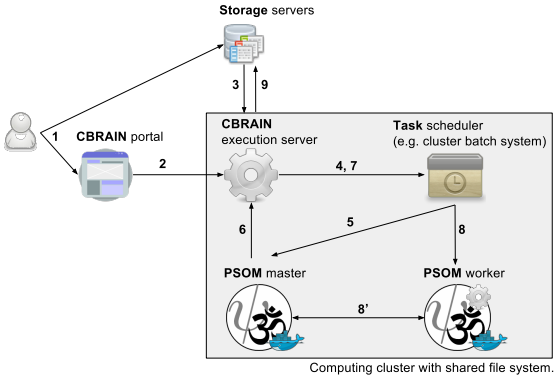
The CBRAIN-FSL integration allows to leverage FSL pipelines written in low-level workflow languages (Linux executables and scripts) that submit tasks uniformly through a specific tool called fsl_sub. It is diagrammed in Figure 4I, where the science gateway is represented by components `CBRAIN portal` and `CBRAIN execution server` and the infrastructure consists of `Storage servers` and `Computing cluster with shared file system`.

The CBRAIN-PSOM integration [36] is shown on Figure 4II. The PSOM workflow engine adopts a pilot-job architecture [45] where a master coordinates workflow execution by submitting workers and establishing direct communication channels with them. Note how this peculiar execution model is totally supported by the sub-tasking architecture.

[8] `http://docs.adaptivecomputing.com`



(I) CBRAIN-FSL integration.



(II) CBRAIN-PSOM integration. Figure reproduced from [36]

Figure 4: CBRAIN architecture for workflow engine integration (sub-tasking). 1: User sends data and workflow execution request to storage server(s) and CBRAIN portal. 2: CBRAIN portal sends execution request to execution server on cluster. 3: Execution server transfers data from storage server(s). 4-5: Execution server starts workflow engine (FSL tool or PSOM master) via task scheduler. 6: Workflow engine submits sub-tasks to execution server (FSL tasks or PSOM agents). 7-8: Execution server starts sub-tasks through task scheduler. 8': (PSOM only) PSOM master and workers execute workflow. 9. Execution server transfers results to storage server(s). Interaction `b` in Figure 2 is implemented by steps `4`, `5`, `7` and `8` (regular interactions with batch manager). Interaction `c` is implemented by steps `3` and `9`. Interaction `e` is implemented by step `6` (for FSL: through a modified version of the fsl_sub script available in `https://github.com/aces/cbrain-plugins-neuro`; for PSOM: through a specific development in PSOM).

2.5. Pool model

See Figure 2(IV). Workflows are submitted by the science gateway to a pool through interaction `d`. Agents connect to the pool asynchronously to retrieve and execute workflows through interaction `f`. Agents may be started according to various policies, for instance to ensure load balancing. Agents may wrap different types of workflow engines. Workflow engine controls tasks and data on the infrastructure through interactions `b` and $\texttt{c}_2$, science gateway transfers user data through interaction $\texttt{c}_1$, and administrator installs workflows through interaction $\texttt{a}_1$ and $\texttt{a}_2$.

The pool model was implemented in the SHIWA pool [37] diagrammed in Figure 5. In this Figure, interaction `d` of Figure 2(IV) is implemented in 3 different types of calls to the pool: workflow submission (`1` & `2`), workflow status retrieval (`0` & `3`), and workflow retrieval (`13` & `14`). In Figure 5, interaction `f` of Figure 2(IV) is implemented through 2 types of calls: workflow instance retrieval (`4`, `5` and `6`), and workflow instance update (`11` and `12`). Workflow instance retrieval is used by the agents to fetch work from the pool. Workflow instance update is used by the agents to update workflow statuses. In the SHIWA pool, agents can wrap different types of workflow engines to execute workflows expressed with different languages. Calls `0`, `7`, `8` and `9` on Figure 5 are used by workflow engine plugins to declare their supported language and launch engines, and by workflow engines to report their status to the agent. These calls are specific to the SHIWA Pool implementation of the `agent` component and therefore have no corresponding representation in Figure 2(IV).

2.6. Nested workflows

See Figure 2(V). In nested workflows (Figure 2(V)-Left), a task of a *parent* workflow executed by the *parent* engine is itself a workflow, called *child* workflow, that is executed by a *child* engine. The parent and child engines might use different workflow description languages. They might also execute workflows on different infrastructures. The parent workflow is also called meta-workflow. The science gateway communicates with the parent engine through abstract interaction $*_1$. The science gateway also communicates with the infrastructure to transfer user data through abstract interactions $*_2$ and $*_3$. Both workflow engines communicate with the infrastructure through abstract interactions $*_4$ and $*_5$. The parent engine communicates with the child engine through abstract interaction

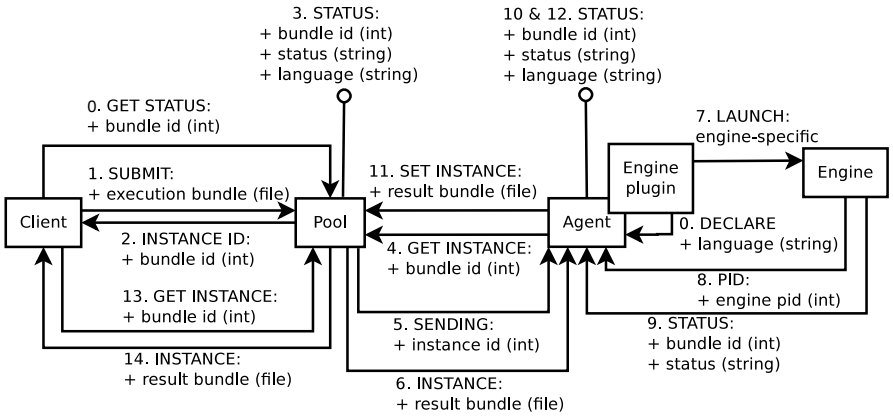


Figure 5: Architecture of the SHIWA pool. Circle-terminated arrows indicate messages that are broadcast to all pool clients. Figure reproduced from [37].

$*_6$. Administrator installs workflows through interactions $\mathtt{a}_1$ and $\mathtt{a}_2$.

Nested workflows are abstract architectural patterns that can be instantiated in the various architectures described previously. We focus on instantiation with the service invocation model (Figure 2(V)-Right) as this is the most used architecture. In such an instantiation, we assume that the parent and child workflow engines are distinct pieces of software that require different workflow services invoked by distinct `d` interactions. If this is not the case, then workflow services can be collapsed in a single one with a `d` interaction with itself. An example of such interaction is the use of hierarchical workflows in Pegasus [7]. Workflow engines communicate with infrastructures using `b` and $\mathtt{c}_2$. Science gateway transfers user data to infrastructures using $\mathtt{c}_1$ interactions.

Nested workflows have long been available in workflow engines, for instance in the Taverna workbench [9]. They are also used implicitly in several platforms where workflow engines are wrapped in workflow tasks as any other command-line tool. Nested workflows were notably used by the SHIWA Science Gateway to implement so-called Coarse-Grained workflow interoperability [27], i.e. to integrate various workflow engines in a consistent platform. Figure 6 shows the architecture used in the SHIWA Simulation Platform for nested workflow execution with service invocation.

2.7. Workflow import

See Figure 2(VI). This is an abstract model instantiated with the service invocation architecture for consistency. Workflows are integrated in the science gateway through format conversion from a native format to the science gateway format. Workflow import is usually an offline process which is not involved in workflow execution. Workflow import was implemented in the SHIWA Simulation Platform through the IWIR language that provided a common language for portability across grid workflow systems [28]. Other systems rely on workflow import. Tavaxy [38] allows to import, merge and run Taverna [9] and Galaxy [48] workflows. When some workflow parts cannot be imported, workflows are run by Tavaxy as nested workflows using their native engine. The work in [39] describes workflow import from KNIME [49] to WS-PGRADE/gUSE and from Galaxy [48] to WS-PGRADE/gUSE.

3. Evaluation

The architectures described in Section 2 are evaluated in Table 2. We use 5 main criteria to evaluate the architectures: global complexity, execution complexity, extensibility, scalability and other specific features. Criteria break down to specific metrics where *lower value indicates better performance*. For each criterion, a total score is computed by summing up the individual metrics. We ensure that the different metrics in a criterion measure similar entities so that they can be summed. The criteria and metrics are explained hereafter.

3.1. Evaluation metrics

Global complexity is obtained by counting the total number of interactions and components on the architecture diagram. It breaks down to the following 2 metrics:

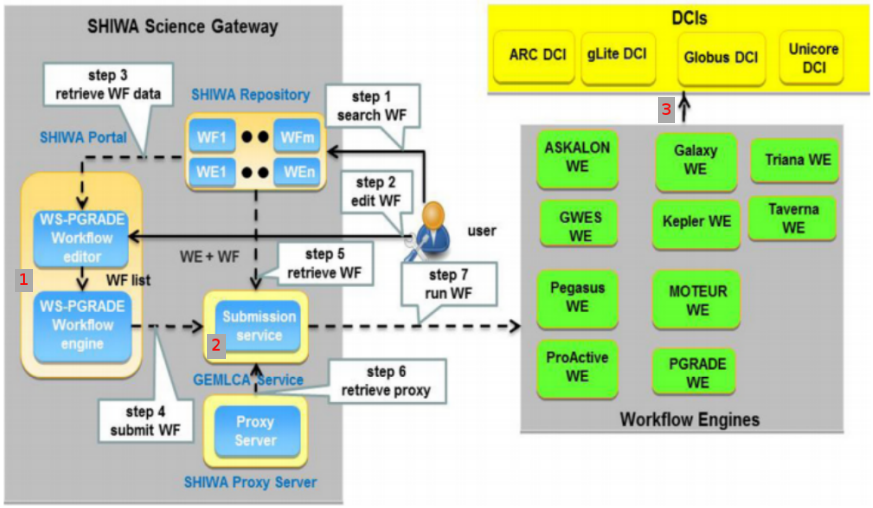


Figure 6: Nested workflow execution through SHIWA Science Gateway. The parent workflow engine is `WS-PGRADE`, invoked as a service in the Science Gateway (step `1`, interaction `d` on Figure 2(V)-Right. Ten different child engines can be used by nested workflows, invoked through the `Submission service` (step `2`, interaction `d`). Each of these engines can submit tasks and transfer data to a distributed computing infrastructure (`DCI`, step `3`, interactions `b` and c_2). Data interactions (`c`) and application porting ones (`a`) are not represented. Figure reproduced from [27] with permission of the first author.

	Tight	Service	Sub-task	Pool	Nested	Import
Global complexity						
Total components – I_1	2	3	2	4	5	3
Total interactions – I_2	5	6	5	7	11	7
Total (total software pieces)	**7**	**9**	**7**	**11**	**16**	**10**
Robustness						
Specific components – R_1	0	1	0	2	2	1
Specific interactions – R_2	2	3	1	4	6	3
Total (execution software pieces)	**2**	**4**	**1**	**6**	**8**	**4**
Extensibility						
New engine type – E_1	3	4	2	3	4.5	1
New engine version – E_2	1	0	1	0	0	1
New workflow – E_3	2	2	2	2	2	3
New infrastructure – E_4	4	4	3	4	6	4
Total (difficulty to extend)	**10**	**10**	**8**	**9**	**12.5**	**9**
Scalability						
Multiple engine instances – S_1	2	1	0	0	1	1
Distributed engines – S_2	1	1	1	1	0	1
Task scheduling – S_3	0	0	1	0	1	0
Total (scalability issues)	**3**	**2**	**2**	**1**	**2**	**2**
Specific features						
Meta-workflow – O_1	1	1	1	1	0	0
Fine-grained debugging – O_2	0	0	1	0	1	0
Total (missing features)	**1**	**1**	**2**	**1**	**1**	**0**

Table 2: Architecture evaluation. Lower values (brighter colors) indicate better performance. On each row, metric values are normalized between 0 (best value) and 1 (worst value) to determine the color of the corresponding table cell. The normalized metric value m' is defined as $\frac{m-m_{\min}}{m_{\min}-m_{\max}}$ where m is the initial metric value, $m_{\min}$ and $m_{\max}$ are the minimal and maximal values among all architectures. The RGB hexadecimal color code of the cell is `#99XX99`, where X=F-4m'.

- Total number of components ($\mathtt{I}_1$), and
- Total number of interactions ($\mathtt{I}_2$).

One may wonder whether infrastructure should be counted in $\mathtt{I}_1$ since it is usually not developed by the groups who integrate workflow engines in science gateway. However, integrating an infrastructure in the architecture usually requires some technical effort (e.g., account creation, software installation, etc.), which is why we keep it in the metric. The two metrics are summed to obtain the total score for global complexity. Global complexity measures the total number of software pieces to develop, including interactions and components. It may be used to measure the development effort required to build the architecture.

Robustness of workflow execution measures the likelihood that workflow execution fails due to errors in the components or with the interactions in the software architecture. Note that errors coming from the infrastructure (e.g., unavailable data or terminated tasks) or workflows (e.g., wrong user input or application errors) are not covered since they do not stem directly from the software architecture. Robustness is measured here as a consequence of global complexity since complex architectures tend to be more prone to failure. More precisely, robustness is determined as the number of software components and interactions that are specific to workflow execution:

- Components ($\mathtt{R}_1$): number of specific components involved in workflow executions. Science gateway, for instance, is *not* specific to workflow execution since it is used to authenticate users, add new workflows, transfer user data, etc.
- Interactions ($\mathtt{R}_2$): number of specific interactions involved in workflow executions.

These specific components and interactions are the ones represented in red in the architecture diagrams in Figure 2. $\mathtt{R}_1$ and $\mathtt{R}_2$ are summed to obtain the total score for this criterion, which measures the total number of software pieces that are specifically involved in the workflow execution.

Extensibility measures the difficulty to replace or add elements in the architecture. It is also a consequence of global complexity and it is determined as the number of interactions and components that need to be modified when a new element is added. Modification of a component is required when its code needs to be updated or recompiled (science gateway or workflow service), or when a new piece of software has to be installed (infrastructure only). Modification of an interaction is deemed necessary when the parameters involved in this interaction are modified. Extensibility breaks down in 4 metrics depending on the type of element that has to be added or replaced:

- New engine type ($\mathtt{E}_1$): number of interactions or components to modify to integrate a new type of workflow engine in the architecture. Workflow engines belong to different types when they cannot be invoked using the same interface. Adding a new type of workflow engine allows to execute more workflows in the science gateway.
- New engine version ($\mathtt{E}_2$): number of interactions or components to modify to integrate a new version of a workflow engine in the architecture, assuming that another version of the same engine type is already available. Different versions of a workflow engine share the same interface, i.e. they can be invoked using the same software. When this is not the case, the different versions are considered as different engine types. Components are not treated equally regarding engine version updates. Components whose only function is to host the workflow engine, i.e. workflow services and agents, are not counted in E_2 because updates in such components are assumed to be straightforward. On the contrary, modifications of components that have other functions than wrapping the engine, i.e. science gateway and infrastructure, are counted in E_2 because updates in these components require more effort, e.g. new release of the science gateway, gaining administrative privileges on the infrastructure, etc.
- New workflow ($\mathtt{E}_3$): adding a new workflow is a very common operation that does not require modifying software components or interactions. We measure the difficulty to integrate a new workflow by counting the number of interactions required to integrate a new workflow in the architecture, assuming that the engine type and version required to execute this workflow are already available.
- New infrastructure ($\mathtt{E}_4$): number of interactions or components to modify to integrate a new type of infrastructure in the architecture. Adding a new infrastructure allows to provide more computing or storage power, to access specific types of resources (e.g., GPUs, clouds), or to enforce execution policies (e.g., constrain data to remain in a particular network domain).

The 4 metrics are summed to obtain a global index that measures the difficulty to extend the architecture. Note that some extensions may involve several metrics in practice. For instance, adding a new type of engine may help integrate new infrastructures when interactions b and c_2 are already present for the new engine and infrastructure.

Scalability corresponds to the ability of the architecture to cope with high workloads. It is measured by counting the potential scalability issues in the architectures, i.e. the lack of scalability features. Features are evaluated using a 3-level metric: 0 means that the feature is very easy to enable, 1 means that it can be implemented but with some difficulty, and 2 means that the feature could only be implemented with a nonsensical amount of effort. Four different features are identified:

• Multiple engine instances (S_1): possibility to have more than 1 engine instance in the architecture. Workflow engines may require important amounts of resources when several workflows, or large workflows, are executed. At some point, it may be required for the science gateway to distribute the load among several engines. S_1=0 when adding a new engine instance is a fully automated process, i.e. the workflow engine only has to be started. In this case, elastic engines are possible, i.e. some kind of auto-scaling mechanism can be implemented to control the number of engine instances in the architecture. S_1=1 when adding a new engine instance requires some form of manual intervention (e.g., two-factor authentication), which prevents easy implementations of elastic engines. S_1=2 when new engine instances cannot be added.

• Distributed engines (S_2): possibility to distribute the execution *of a single workflow* among different engine instances. In our scope, this feature focuses on the capabilities of the architecture rather than these of the workflow engine. S_2=0 when distributed engines are possible in the architecture, S_2=1 when they require specific developments in the workflow engine..

• Task scheduling (S_3): task scheduling is a difficult issue that depends more on the implementation of specific algorithms in the science gateway, workflow engine and infrastructure than on the architecture used to integrate the workflow engine in the science gateway. Some architectures, however, complexify the task scheduling problem by introducing additional software layers or create tasks with specific characteristics. S_3=0 when the architecture does not introduce any additional complexity to the scheduling problem, and S_3=1 otherwise.

The 3 metrics are summed to obtain a global measure of the scalability issues that are present in the architecture.

Specific features include:

• Meta-workflow (O_1): ability to describe meta-workflows from existing workflows. Meta-workflows offer an additional level of flexibility to build workflows from reusable components. O_1=0 when the feature is available, O_1=1 otherwise.

• Fine-grained debugging (O_2): availability of fine-grained debugging information about workflow tasks (white-box workflow). Fine-grained information about workflow tasks is required to properly troubleshoot workflow executions. O_2=0 when such information is easy to access, O_2=1 otherwise.

O_1 and O_2 are summed to obtain a total number of missing specific features in the architecture.

The architectures described in Figure 2 are evaluated along these metrics in the remainder of this Section.

3.2. Tight integration

Global complexity. This architecture does not require any component in addition to the science gateway and infrastructure (I_1=2). It involves 5 interactions: a_1, a_2, b, c_1 and c_2 (I_2=5).

Robustness. No component is specific to workflow execution (R_1=0), but interactions b and c_2 are (R_2=2).

Extensibility. Integrating a new type of workflow engine requires to modify the science gateway as well as interactions b and c_2 (E_1=3). Updating a workflow engine version requires modifications in the science gateway (E_2=1). Inserting a new workflow is done through interactions a_1 and a_2 (E_3=2). Adding a new infrastructure generates updates in interactions a_1, b, c_1 and c_2 (E_4=4).

Scalability. Adding a new engine instance requires a new instance of the science gateway, which is in general not possible (S_1=2). Specific IT setups such as load-balancing between web server instances might be used to deal with this issue. Distributed engines are not available by default

(S_2=1). The scheduling of tasks on the infrastructure is as complex as in any other architecture since the workflow engine might implement any kind of scheduling policy (S_3=0).

Specific features. Meta-workflows are not supported by default (O_1=1). Debugging is not an issue since the science gateway can retrieve any information from the workflow engine directly (O_2=0).

3.3. Service invocation

Global complexity. Service invocation requires a workflow service in addition to the science gateway and infrastructure (I_1=3). The architecture involves 6 interactions: a_1, a_2, b, c_1, c_2 and d (I_2=6).

Robustness. The workflow service is a component specific to workflow execution (R_1=1). Workflow execution also involves 3 specific interactions: b, c_2 and d (R_2=3).

Extensibility. Adding a new type of workflow engine requires to implement the corresponding workflow service, to modify interaction d, and to implement interactions b and c_2 (E_1=4). New engine versions can be added by updating the workflow service without modifying any interaction or component (E_2=0). Updating the engine version in a workflow service does not count since the only goal of this component is to wrap the engine. New workflows are added in the science gateway or in the workflow engine through interactions a_1 and a_2 (E_3=2). Adding a new type of infrastructure requires updates in interactions a_1, b, c_1 and c_2 (E_4=4).

Scalability. The service architecture supports multiple engine instances through multiple workflow services. In VIP for instance, this feature has been available from release 1.17 (April 2016). A basic load-balancing mechanism is available that sends new workflow executions to the engine instance that has the least active executions. To avoid "black-hole" syndromes created by failing engine instances, engine instances are automatically disabled when workflows cannot be submitted to them. Adding a new engine instance, however, requires manual intervention to declare the new instance in the science gateway (S_1=1). Consequently, elastic engines are difficult to implement because they require a mechanism to update the science gateway configuration when a new engine instance is available. Distributing the execution of a single workflow in multiple engines is usually not possible unless the workflow engine has specific abilities (S_2=1). The scheduling of tasks on the infrastructure is as complex as in any other architecture since the workflow engine might implement any kind of scheduling policy (S_3=0).

Specific features. Meta-workflows are not supported by default (O_1=1). Fine-grained debugging information is usually easy to obtain since the workflow service provides direct access to the engine (O_2=0).

3.4. Sub-task

Global complexity. The sub-task architecture requires only 2 components (I_1=2). It involves 5 interactions: a_1, a_2, b, c and e (I_2=5).

Robustness. No component is specific to workflow execution (R_1=0), and only interaction e is (R_2=1).

Extensibility. Integrating a new type of workflow engine requires to develop interaction e and to install the engine on the infrastructure (E_1=2). Updating an engine version requires updates only on the infrastructure (E_2=1). New workflows are integrated by creating a new task in the science gateway through interactions a_1 and a_2 (E_3=2). Adding a new infrastructure requires to update interactions a_1, b and c in the science gateway (E_4=3).

Specific features. Meta-workflows are not available (O_1=1). Obtaining fine-grained information about workflow tasks is not straightforward since the science gateway has no knowledge about the workflow topology, and the workflow engine is integrated as a task (O_2=1).

Scalability. New engine instances are spawned and executed on the infrastructure as any other task upon user submission (S_1=0). This is a major interest of the sub-task architecture. Distributed engines are not supported by default (S_2=1). Task scheduling is slightly more complex than in the other approaches due to the special role of the task that executes the workflow engine (S_3=1). Indeed, the reliability of this task is critical since all the sub-tasks in the workflow depend on it and, depending on the recovery capabilities of the workflow engine, may need to be resubmitted if the workflow task fails. The workflow task is also longer than all its sub-tasks, which increases its chances of failure. In addition, task parameters, for instance estimated walltime, are more difficult to estimate for

the workflow task than for sub-tasks which may generate issues such as selection of wrong batch queues on clusters. Finally, the interdependencies between the workflow task and its sub-tasks may create deadlocks when there is contention. For instance, if only 1 computing resource is available for the science gateway and that the workflow task is running on it and submits sub-tasks, then the sub-tasks could only execute when the resource is available, which will never happen because the workflow task will not complete until the sub-tasks complete. This configuration can be generalized to an infrastructure with n resources where n workflows are submitted. In practice, however, the number of submitted workflows usually remains lower than the number of computing resources available on this infrastructure, which makes such deadlocks unlikely to happen.

3.5. Pool

Global complexity. The pool model requires a workflow pool and an agent in addition to the science gateway and infrastructure (I_1=4). It involves 7 interactions: a_1, a_2, b, c_1, c_2, d and f (I_2=7).

Robustness. The workflow pool and agent are specific to workflow execution (R_1=2). Interactions b, c_2, d and f also are (R_2=4).

Extensibility. Adding a new engine type requires to wrap the engine in the agent and to update interactions b and c_2 (E_1=3). Updating the version of an engine is transparent (E_2=0) since it only requires updating the agent that is a component dedicated to the engine. Integrating a new workflow is done through interactions a_1 and a_2 (E_3=2). Integrating a new infrastructure requires updates in interactions a_1, b, c_1 and c_2 (E_4=4).

Scalability. New engine instances only require new agents, which is easily automated (S_1=0) and by design very suitable for elastic computing. For instance, auto-scaling rules can be implemented to start new agents when the workload in the science gateway exceeds a certain threshold [50]. Distributed engines are not available by default (S_2=1) and task scheduling is as complex as in any other architecture (S_3=0).

Specific features. Meta-workflows are not available by default (O_1=1). Accessing debugging information is not likely to be an issue since the workflow pool could implement specific functions for that (O_2=0).

3.6. Nested workflows with service invocation

Global complexity. Setting up a nested workflow architecture with service invocation requires a science gateway, 2 workflow services and 2 infrastructures (I_1=5). The architecture involves 11 interactions (I_2=11): a_1 (appears twice: once for each infrastructure), a_2, b (twice: once for each infrastructure), c_1 (twice: once for each infrastructure), c_2 (twice: once for each workflow engine and infrastructure) and d (twice: once for each workflow engine).

Robustness. The two workflow services are specific to workflow execution (R_1=2). Interactions b (counted twice), c_2 (twice) and d (twice) also are (R_2=6).

Extensibility. Adding a new type of *parent* engine requires to implement the corresponding service, to implement interactions b and c_2 in the parent engine, and to implement interaction d in the science gateway and in the parent service (E_1=5). Adding a new type of *child* engine only requires to implement the corresponding service, to develop interactions b and c_2 in the child engine, and to implement interaction d in the parent service (E_1=4). We use E_1=4.5 in Table 2 to reflect both conditions. Adding a new version in the parent or child engine only requires modifying this engine (E_2=0). Adding a new workflow is done through interaction a_1 and a_2 (E_3=2). Adding a new infrastructure requires to re-implement interactions a_1, b and c_2 twice, and interaction c_1 once (E_4=6).

Scalability. As in the service architecture, adding a new workflow instance requires manual configuration in the science gateway (instance of a parent engine), or in the parent engine (instance of a child engine) (S_1=1). Similarly, elastic engines are difficult to achieve. Distributed engines are possible, through meta-workflows (S_2=0). Task scheduling is more complex than in other architectures though, due to the fact that workflow execution is split in different engines (S_3=1).

Specific features. Meta-workflows are possible, which is one of the main interest of this architecture (O_1=0). Debugging is difficult because the science gateway cannot directly access fine-grained information in the sub-workflow (O_2=1).

3.7. Workflow import with service invocation

Global complexity. Workflow import with service invocation requires the same components as for service invocation (I_1=3). It requires an additional g interaction for workflow import (I_1=7).

Robustness. Since workflow conversion is not involved in the execution (it is an offline process), metrics are as in the service architecture (R_1=1, R_2=3).

Extensibility. Since adding a new type of workflow engine aims at supporting more workflows, we consider that it only requires to re-implement interaction g in this architecture (E_1=1). Note, however, that implementing interaction g can require very substantial work depending on the complexity of the language used by the new engine. Based on the same logic, adding a new engine version only requires modifying interaction g (E_2=1). Adding a new workflow is done through interactions a_1, a_2 and g (E_3=3). As in the service architecture, interfacing with a new infrastructure requires modifications in the workflow service and in interactions a_1, b and c_2 (E_4=4).

Scalability. Since workflow conversion is not involved in the execution (it is an offline process), metrics are as in the service architecture (S_1=1, S_2=1, S_3=0).

Specific features. Meta-workflows are available after import, by connecting workflows in the language used in the science gateway (O_1=0). Debugging information is accessible as in the service invocation architecture (O_2=0).

4. Discussion

4.1. Comparison between architectures

Tight integration and sub-tasking are globally the simplest architectures, followed by service integration, workflow import (with service invocation) and pool. Nested workflows (with service invocation) requires more integration than the other architectures. Robustness roughly leads to the same ordering of architectures, with tight integration and sub-tasking in the top group, service integration and workflow import (with service invocation) close behind, pool in a third group, and nested workflows (with service invocation) at the end. This ordering is consistent across metrics, it reflects the global complexity of the architectures.

Regarding extensibility, most architectures are overall comparable, except nested workflows (with service invocation) which is significantly behind. This is explained by the complexity of the nested workflow architecture, with 2 infrastructures and 2 workflow services. Sub-tasking and workflow import (with service invocation) perform a bit better when integrating new engines (E_1), which is interesting given the current profusion of engines with different characteristics. However, sub-tasking, workflow import (with service invocation) and tight integration perform worse than the others when adding engine versions (E_2) due to the need to update infrastructure (sub-tasking), science gateway (tight integration), or workflow converter (workflow import). Workflow import performs worse than the others when integrating new workflows (E_3) because of the language conversion step. All architectures except nested workflows perform the same when integrating new infrastructures (E_4).

The pool architecture is overall the most scalable, which is not a surprise since it was designed precisely for scalability. Tight integration is the least scalable and all the other architectures perform the same. The overall scalability score, however, should not mask the unique characteristics of architectures regarding this criterion. Nested workflows are the only architecture that can easily accommodate distributed workflow execution, which can be critical in some cases. At the same time, the scheduling constraints created by the sub-tasking and nested workflow architectures could well become showstoppers depending on the type of the targeted infrastructure. Non-reliable infrastructures, for example, could hardly cope with workflow engines being wrapped in computing tasks as done in sub-tasking. The availability of multiple engine instances could also become a critical feature for science gateways with important workloads, which would favor sub-tasking and pool.

Differences in other specific features should not be neglected. Nested workflows (with service invocation) and workflow import (with service invocation) are the only architectures that support meta-workflows, which may be interesting in some cases. Also, sub-tasking and nested workflows may complexify fine-grained debugging. The availability of fine-grained debugging information may also be critical to efficient user support.

Table 3 provides an overall comparison between

	Tight	Service	Sub-task	Pool	Nested	Import
Global complexity (normalized total)	0.00	0.22	0.00	0.44	1.00	0.33
Robustness (normalized total)	0.14	0.43	0.00	0.71	1.00	0.43
Extensibility (normalized total)	0.44	0.44	0.00	0.22	1.00	0.22
Scalability (normalized total)	1.00	0.50	0.50	0.00	0.50	0.50
Specific features (normalized total)	0.50	0.50	1.00	0.50	0.50	0.00
	2.1	**2.1**	**1.5**	**1.9**	**4.0**	**1.5**

Table 3: Overall evaluation. Brighter colors and lower scores indicate better performance. Scores are obtained by summing the normalized total scores (m' values) of each criterion in Table 2 and the colors are obtained by normalizing these scores as done in Table 2.

architectures, based on the metrics in Table 2. Note that this analysis is only for illustration purposes since it assumes that all criteria have equal weights while real systems would favor some of them. Overall, sub-tasking, and workflow import (with service invocation) perform a bit better than tight integration, service invocation and pool. Nested workflows stands a bit behind for the reasons mentioned previously.

4.2. Limitations

A few limitations remain that should be considered when using the results of our evaluation. First of all, the evaluation is done at a quite high-level of abstraction that may be a bit artificial when applied to real systems. Abstracting architectures from their implementation in specific systems is useful to compare them, but we also realize that this comes at the cost of realism. In particular, the presented architectures are theoritical patterns that may be blended in actual systems. The distinction between tight integration and service invocation, for instance, may not be always that clear in practice. Service invocation may also be combined with sub-tasking in some cases. However, the criteria discussed in this work would still apply to broadly compare and categorize such cases of hydrid architectures.

Moreover, all the interactions involved in the architectures were treated equally while some of them are obviously more complex than others. For example, interaction `g` (workflow language conversion) is clearly more complex than interaction `d` (service invocation), and may create much more reliability issues as well. However, quantifying the robustness and amount of development associated with each interaction and software component cannot realistically be done without entering into the details of a particular system.

The particular case of interaction `g` (workflow language conversion) should be further discussed since it is very likely that this interaction could not be easily generalized to any workflow language. For instance, converting FSL, PSOM or Nipype pipelines to any other workflow language is problematic because these engines rely on general-purpose programming languages such as Bash, Octave and Python, which are much richer than scientific workflow languages.

The abstract nested workflows and workflow import patterns were instantiated with service invocation so that they can be analyzed in the same framework as the other architectures. Other types of instantiation, for instance nested workflows with sub-tasking, could also be envisaged. We chose to limit ourselves to instantiations with service invocation because the resulting architectures are implemented in real systems, and because service invocation is largely used. Nested workflows with sub-tasking, in particular, could be an interesting architecture to explore.

Finally, the particular technical or historical context of a science gateway project may obviously influence the choice of an architecture to integrate workflow engines. For instance, some workflow engines may be already available as web services, which would tend to favor service invocation, and other science gateways may have strongly tested task and data control features (interactions `b` and `c`), which would favor sub-tasking. Similarly, adding a new type of engine may facilitate integration of a new infrastructure when interactions `b` and $\mathtt{c}_2$ are already available. The migration cost between architectures has been ignored as well.

5. Conclusion

We reviewed architectures used to integrate workflow engines in science gateways, we described them in a system-independent framework suitable for comparison, we illustrated them on real systems, we developed quantitative metrics for evaluation,

we evaluated these metrics for all the architectures, and we discussed the pros and cons of all the architectures based on these metrics.

To the best of our knowledge, our work is the first of its kind. Our results can be used as recommendation for science gateway and workflow engine architects to build new platforms, or to upgrade existing ones.

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