Software architectures to integrate workflow engines in science gateways

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Abstract

We investigate six software architectures commonly used to integrate workflow engines in science gateways. In *tight integration*, the workflow engine shares software components with the science gateway. In *service invocation*, the engine is isolated and invoked through a specific software interface. In *task encapsulation*, the engine is wrapped as a computing task executed on the infrastructure. In the *pool model*, the engine is bundled in an agent that connects to a central pool to fetch and execute workflows. In *nested workflows*, the engine is integrated as a child process of another engine. In *workflow import*, the engine is integrated through workflow language conversion. We describe and evaluate these architectures with metrics that measure integration complexity, robustness, extensibility, scalability and support for meta-workflows and fine-grained debugging. Results provide insights for science gateway architects and workflow engine developers. Tight integration and task encapsulation are the easiest to integrate and are most robust. Extensibility is equivalent in most architectures. The pool model is the most scalable one and meta-workflows are only available in nested workflows and workflow import.

Keywords: Workflow engines, science gateways, software architectures.

1. Introduction

Workflow engines are critical for the efficient and transparent exploitation of distributed infrastructures in the ecosystem of tools and services offered by science gateways. Several software architectures can be adopted to integrate workflow engines in science gateways, with important consequences on the development effort required and resulting system.

This paper describes, provides examples and compares such architectures, based on system-independent representations of their main components and interactions. It is informed by our experince in the development and sustained operation of the CBRAIN [37] and VIP [16] science gateways for medical image analysis during the past 7 years; as well as by lessons learned from several science gateway and workflow projects such as SHIWA[1].

In this section we provide background information and definitions of workflow engines, science gateways and infrastructures. In Section 2, we describe six architectures within a consistent framework that underlines the functional interactions between their main software components. In Section 3, the different architectures are evaluated with metrics measuring integration complexity, robustness, extensibility, scalability and other specific features. We finally compare the architectures and highlight recommendations for science gateway architects and workflow engine developers.

1.1. Workflow engines

In the last decade, the e-Science community has developed workflow systems to help application developers access distributed infrastructures such as clusters, grids, clouds and web services. These efforts resulted in tools among which Askalon [15], Hyperflow [5], MOTEUR [17], Pegasus [11, 12],

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

Swift [44], Taverna [31], Triana [39], VisTrails [8] and WS-PGRADE [25]. Such workflow engines usually describe applications in a high-level language with specific data and control flow constructs, parallelization operators, visual edition tools, links with domain-specific application repositories, provenance recording and other features. An overview of workflow system capabilities is available in [10].

At the same time, toolboxes have been 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 [21]), PSOM (Pipeline System for Octave and Matlab [6]), PMP (Poor Man's Pipeline [2]), RPPL [45], SPM (Statistical Parametric Mapping [4]) and FSL (FMRIB Software Library [23]) 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 infrastructures, in particular clusters, to execute tasks at a high throughput. Some of these tools also support advanced features such as provenance tracking, or redundancy detection across analyses to avoid re-computation. A wide array of workflows have been implemented using these pipeline systems and are now shared across neuroimaging groups world-wide, which represents a tremendous opportunity for science gateways to leverage. Domain-specific engines nicely complement e-Science systems that are more oriented towards the exploitation of distributed computing infrastructures, in particular grids and clouds.

In this paper, a *workflow engine* (also abbreviated *engine*) is 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*), using input data that may consist of files, database entries or simple parameter values. Although simplistic, this definition covers both e-Science workflow systems and domain-specific pipeline systems. 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 within 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.

Various science gateways have been developed, including frameworks such as Apache Airavata [29], the Catania Science Gateway Framework [3] and WS-PGRADE/gUSE [25]. Numerous science gateways were built using such frameworks [24, 3] or as standalone systems [37, 16]. Most of these systems include one or several workflow engines.

Integration between workflow engines and science gateways varies across systems. Some science gateways are tailored to a particular engine, while other ones are more general and host applications executed by different types of engines.

Extensibility is an important property of the integration. 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 a crucial concern for such multi-user, high-throughput systems. For this purpose, science gateways may balance the load among different instances of the same engine, start new engines elastically using auto-scaling techniques such as the ones reviewed in [27], and use advanced task scheduling policies on the infrastructure to improve performance, fault-tolerance and fairness among users.

Robustness is highly desirable as well since it is key to a good user experience. Simple architectures facilitate the implementation effort towards robust interactions which, in turn, have a positive impact on characteristics such as gateway predictability, transparency, reliability, traceability and reproducibility.

Other specific features may also be available, for instance data vizualisation and quality control, workflow edition, debugging instruments, or social tools among users.

1.3. Infrastructure

Infrastructure consists of the computing and storage resources involved in workflow execution, as

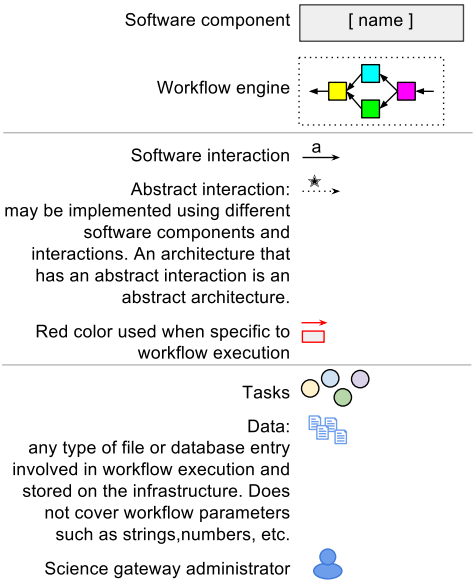


Figure 1: Graphical notations

well as the software services used to access these resources. Infrastructure can be composed of computing or file servers, databases, clusters, grids or clouds. Some workflow engines and science gateways may require specific characteristics, 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 requirements 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. 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 as in Figure 2.

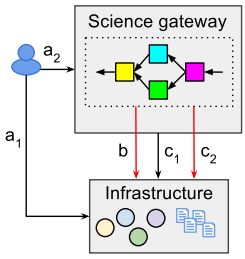
(a) Workflow integration: consists in adding a new workflow to the system so that users can execute it. It is triggered by an administrator of the science gateway and it results in an interface, for instance a web form, where users can enter the parameters of the workflow to be executed. The interaction has two steps: (a_1) the programs used in the workflow are installed on the infrastructure, which may require administrative privileges; (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 [20]), DRMAA (Distributed Resource Management Application API [41]), or OCCI (Open Cloud Computing Interface [14]).

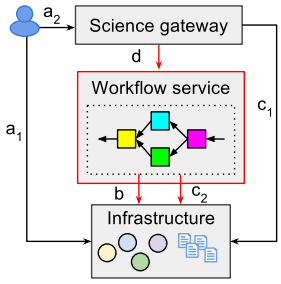
(c) Data control: operations to manage data on the infrastructure, such as: upload, download, deletion, browsing, replication, caching, etc. Data movements can be triggered by the user in the science gateway (c_1), to upload input data or download processed data. They can also be performed by the workflow 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. Tools and services such as JSAGA [34] or Data Avenue [22] 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, dependencies and so on.

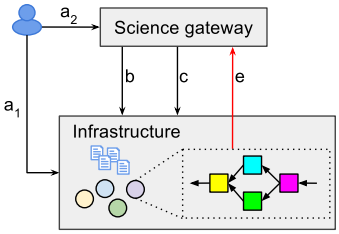
(e) Sub-task control: operations used by tasks to submit sub-tasks on the infrastructure, including: submission, monitoring, termination, deletion, etc. Sub-task control is similar to interaction b, except



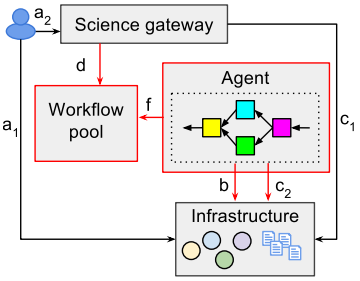
(I) Tight integration



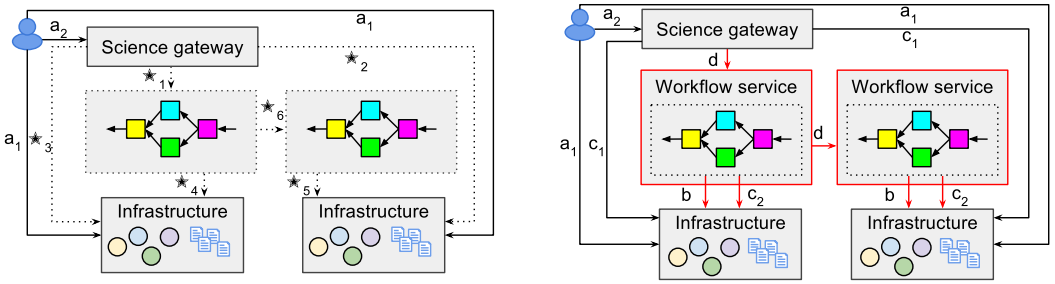
(II) Service invocation



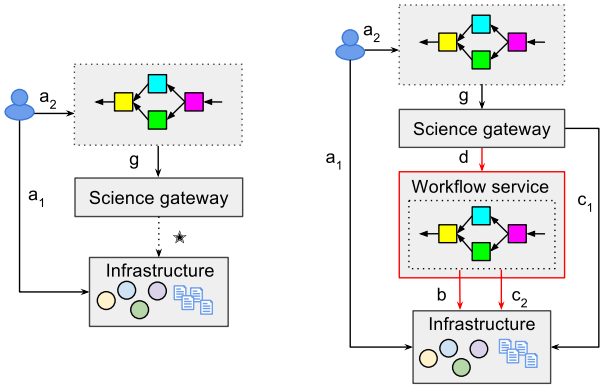
(III) Task encapsulation



(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 [3], Distributed application runtime environment (DARE [28]), DECIDE [3]^{c,n}, LONI Pipeline Environment^{n} [13]
Service	Apache Airvata [29], e-BioInfra [36]^{w,n}, HubZero with Pegasus [30], MoSGrid [26]^{w}, System in [43], Vine Toolkit [38], Virtual Imaging Platform [16]^{n}, WS-PGRADE/gUSE framework [25], Science gateways in [24]^{w}
Task	CBRAIN and PSOM [18]^{n}, CBRAIN and FSL^{n}
Pool	SHIWA pool [35]
Nested	SHIWA Simulation Platform (Coarse-Grained Interoperability [40])^{w}, HubZero with Pegasus (via hierarchical workflows) [12], Tavaxy [1].
Import	SHIWA Simulation Platform (Fine-Grained Interoperability) [33]^{w}, Tavaxy [1], system in [9].

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.

that information about the parent of 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 [42] 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 languages such as between GWorkflowDL and Scufl [32], and between the 4 languages that were involved in the SHIWA initiative.

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 model in a Ruby on Rails application. The workflow engine and the science gateway usually share a database where applications, 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 [3] (see specific documentation on workflows[2]), in the Distributed application runtime environment (DARE) [28], in Galaxy [19], and in the LONI Pipeline Environment [13]. 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, as 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 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 [29], Vine Toolkit [38], Virtual Imaging Platform [16], the system in [43] and the WS-PGRADE/gUSE framework [25]. The integration between the HubZero science gateway and

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

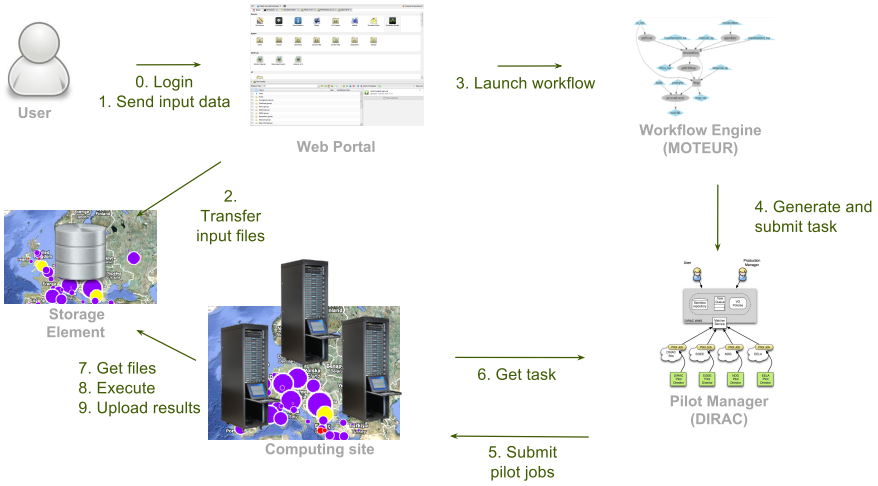


Figure 3: Architecture of the Virtual Imaging Platform (service invocation). Step 3 corresponds to interaction d in Figure 2(II), step 2 corresponds to interaction c_1, step 4 maps to interaction b, and steps 7 and 9 map to c_2 (in VIP, workflow data transfers are performed by the tasks and embedded in their descriptions).

the Pegasus workflow engine performed in [30] 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 [17] is invoked through a service.

2.4. Task encapsulation

See Figure 2(III). The workflow engine is wrapped in 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 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 cluster managers (see for instance attribute `depend` of option `-W` in Torque[3]).

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.

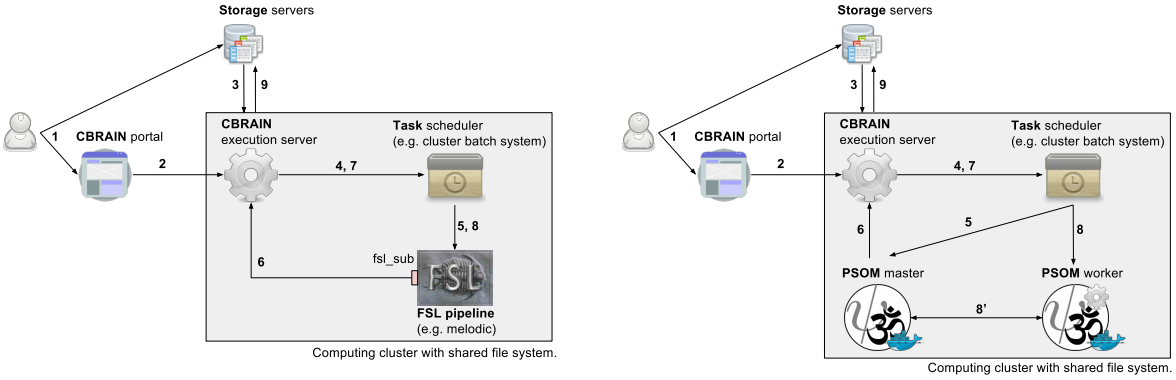
[3] `http://docs.adaptivecomputing.com`

Task encapsulation is implemented in CBRAIN [37] where it is used to integrate the FSL toolkit [23] and the PSOM workflow engine [6]. 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 4(I), 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 [18] is shown in Figure 4(II). The PSOM workflow engine adopts a pilot-job architecture [42] where a master coordinates workflow execution by submitting workers and establishing direct communication channels with them. Note how this peculiar execution model is well supported by task encapsulation.

2.5. Pool model

See Figure 2(IV). Workflows are submitted by the science gateway to a central 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. Workflow engine controls tasks and data on the infrastructure through interactions b and c_2, science gateway transfers user data through interaction c_1,



(I) CBRAIN-FSL integration.

(II) CBRAIN-PSOM integration. Figure reproduced from [18].

Figure 4: CBRAIN architecture for workflow engine integration (task encapsulation). 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 (FSL sub-tasks or PSOM workers). FSL sub-tasks will run locally instead of being submitted again to CBRAIN through interaction 6. 8': (PSOM only) PSOM master and workers execute workflow. 9. Execution server transfers results to storage server(s). Interaction `b` in Figure 2(III) 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).

and administrator installs workflows through interaction $\mathtt{a}_1$ and $\mathtt{a}_2$.

The pool model was implemented in the SHIWA pool [35] diagrammed in Figure 5, where agents can wrap different types of workflow engines to execute workflows expressed with different languages.

2.6. Nested workflows

See Figure 2(V). In nested workflows (Figure 2(V)-Left), workflows include other workflows that are executed by a *child* engine. Parent and child engines might use different languages and might run on different infrastructures. A 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 $*_6$. 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 the 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 [12]. 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 [31]. 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 [40], 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.

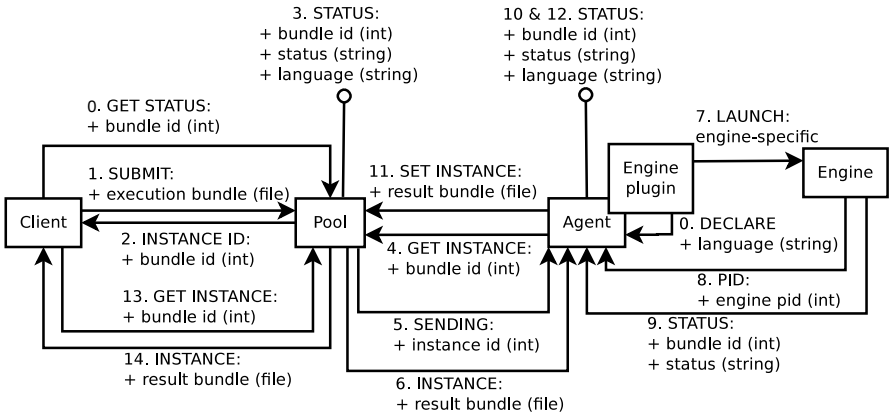


Figure 5: Architecture of the SHIWA pool. Circle-terminated arrows indicate messages that are broadcast to all pool clients. Interaction `d` of Figure 2(IV) is implemented by 3 different calls to the pool: workflow submission (`1` & `2`), workflow status retrieval (`0` & `3`), and workflow retrieval (`13` & `14`). Interaction `f` 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. Calls `0`, `7`, `8` and `9` are used by workflow engine plugins to declare their supported language and to 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). Figure reproduced from [35].

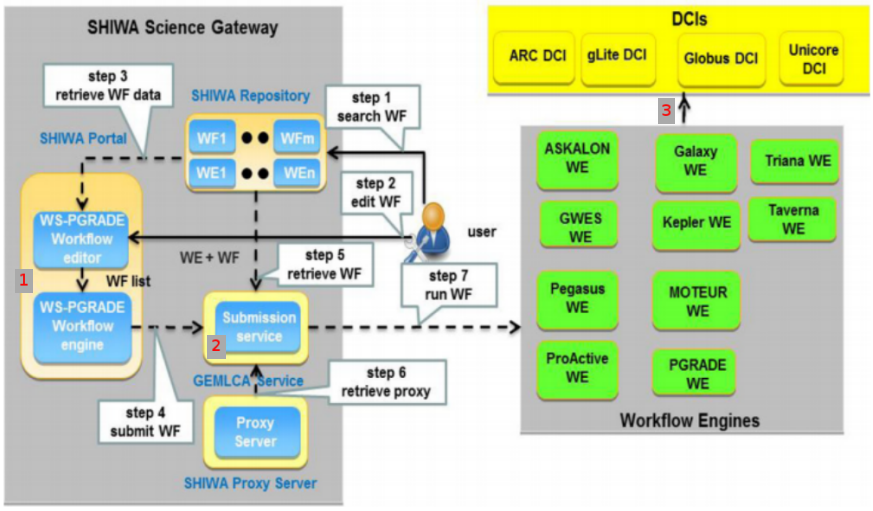


Figure 6: Nested workflow execution through SHIWA Science Gateway. The parent workflow engine is `WS-PGRADE`, invoked as a service in the Science Gateway (step `1`, interaction `d` on Figure 2(V)-Right). Ten different child engines can be used by nested workflows, invoked through the `Submission service` (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). User data interactions (c_1) and application porting ones (`a`) are not represented. Figure reproduced from [40] with permission of the first author.

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 that is not involved in workflow execution. A few systems have implemented workflow import. In the SHIWA Simulation Platform, it is implemented through the IWIR language that provides a common language for portability across grid workflow systems [33] and allows to convert among n workflow languages using $2n$ interactions instead of n^2. Tavaxy [1] allows to import, merge and run Taverna [31] and Galaxy [19] workflows; when some workflow parts cannot be imported, workflows are run by Tavaxy as nested workflows using their native engine. The work in [9] describes workflow import from KNIME [7] to WS-PGRADE/gUSE and from Galaxy [19] to WS-PGRADE/gUSE.

3. Evaluation

The architectures described in Section 2 are evaluated in Table 2 using 5 main criteria: integration complexity, robustness, extensibility, scalability and other specific features. Criteria break down to specific metrics where *lower value indicates better performance*. For each criterion, a global 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

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

- 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, APIs, etc.), which is why we keep it in the metric. The two metrics are summed to obtain a global score that measures the total number of software pieces to develop, including interactions and components.

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. 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 global 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 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 to 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.

	Tight	Service	Task	Pool	Nested	Import
Integration complexity						
Total components – $\mathtt{I}_1$	2	3	2	4	5	3
Total interactions – $\mathtt{I}_2$	5	6	5	7	11	7
Total (total software pieces)	**7**	**9**	**7**	**11**	**16**	**10**
Robustness						
Specific components – $\mathtt{R}_1$	0	1	0	2	2	1
Specific interactions – $\mathtt{R}_2$	2	3	1	4	6	3
Total (execution software pieces)	**2**	**4**	**1**	**6**	**8**	**4**
Extensibility						
New engine type – $\mathtt{E}_1$	3	4	2	3	4.5	1
New engine version – $\mathtt{E}_2$	1	0	1	0	0	1
New workflow – $\mathtt{E}_3$	2	2	2	2	2	3
New infrastructure – $\mathtt{E}_4$	4	4	3	4	6	4
Total (difficulty to extend)	**10**	**10**	**8**	**9**	**12.5**	**9**
Scalability						
Multiple engine instances – $\mathtt{S}_1$	2	1	0	0	1	1
Distributed engines – $\mathtt{S}_2$	1	1	1	1	0	1
Task scheduling – $\mathtt{S}_3$	0	0	1	0	1	0
Total (scalability issues)	**3**	**2**	**2**	**1**	**2**	**2**
Specific features						
Meta-workflow – $\mathtt{O}_1$	1	1	1	1	0	0
Fine-grained debugging – $\mathtt{O}_2$	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. Cell color is set as follows: (1) on each row, metric values are normalized between 0 (best value) and 1 (worst value): $m' = \frac{m - m_{\min}}{m_{\max} - m_{\min}}$ where m is the metric value, $m_{\min}$ and $m_{\max}$ are the minimal and maximal values among all architectures; (2) the RGB hexadecimal color code of the cell is `#99XX99`, where X=`round`(F-6m') (`round` rounds a number to the nearest integer).

• 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 $\mathtt{b}$ and $\mathtt{c}_2$ 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 missing 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 cannot realistically be implemented. 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, complicate the task scheduling problem by introducing additional software layers or creating 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

Integration 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

Integration 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 ($\mathtt{R}_1$=1). Workflow execution also involves 3 specific interactions: `b`, $\mathtt{c}_2$ and `d` ($\mathtt{R}_2$=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 ($\mathtt{E}_1$=4). New engine versions can be added by updating the workflow service without modifying any interaction or component ($\mathtt{E}_2$=0). Updating the engine version in a workflow service does not count in $\mathtt{E}_2$ 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 $\mathtt{a}_1$ and $\mathtt{a}_2$ ($\mathtt{E}_3$=2). Adding a new type of infrastructure requires updates in interactions $\mathtt{a}_1$, `b`, c_1 and c_2 ($\mathtt{E}_4$=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. A basic load-balancing mechanism is available that sends new workflow executions to the engine instance which 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 ($\mathtt{S}_1$=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 ($\mathtt{S}_2$=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 ($\mathtt{S}_3$=0).

Specific features. Meta-workflows are not supported by default ($\mathtt{O}_1$=1). Fine-grained debugging information is usually easy to obtain since the workflow service provides direct access to the engine ($\mathtt{O}_2$=0).

3.4. Task encapsulation

Integration complexity. Task encapsulation requires only 2 components ($\mathtt{I}_1$=2). It involves 5 interactions: $\mathtt{a}_1$, $\mathtt{a}_2$, `b`, `c` and `e` ($\mathtt{I}_2$=5).

Robustness. No component is specific to workflow execution ($\mathtt{R}_1$=0), and only interaction `e` is ($\mathtt{R}_2$=1).

Extensibility. Integrating a new type of workflow engine requires to develop interaction `e` and to install the engine on the infrastructure ($\mathtt{E}_1$=2). Updating an engine version in the architecture shares the same mechanism as version updates of other tasks, which requires an update on the infrastructure ($\mathtt{E}_2$=1). New workflows are integrated by creating a new task in the science gateway through interactions $\mathtt{a}_1$ and $\mathtt{a}_2$ ($\mathtt{E}_3$=2). Adding a new infrastructure requires to update interactions $\mathtt{a}_1$, `b` and `c` in the science gateway ($\mathtt{E}_4$=3).

Scalability. New engine instances are spawned and executed on the infrastructure as any other task upon user submission ($\mathtt{S}_1$=0). This is a major interest of task encapsulation. Distributed engines are not supported by default ($\mathtt{S}_2$=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 ($\mathtt{S}_3$=1). Indeed, the reliability of this task is critical since all the subtasks 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 the sub-tasks because workflows are by definition more complex than their sub-tasks: errors on sub-task parameter estimations accumulate in the workflow, and additional control constructs such as tests and loops may further increase the uncertainty. Such parameter estimation errors may generate issues such as selection of wrong batch queues on clusters or task termination due to exceeded quotas. 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 if 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.

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).

3.5. Pool model

Integration 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 [27]. 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

Integration 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 (twice), a_2, b (twice), c_1 (twice), c_2 (twice) and d (twice).

Robustness. The two workflow services are specific to workflow execution (R_1=2). Interactions b (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 so that it can be supported by both workflow engines (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

Integration 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. Similarly, 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 interactions a_1, b, c_1 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 task encapsulation are the simplest architectures to integrate, followed by service integration, workflow import (with service invocation) and pool. Nested workflows (with service invocation) require more integration than the other architectures. Robustness roughly leads to the same ordering of architectures, with tight integration and task encapsulation 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 are significantly behind. This is explained by the complexity of the nested workflow architecture, with 2 infrastructures and 2 workflow services. Task encapsulation and workflow import (with service invocation) perform slightly better when integrating new engines (E_1), which is interesting given the current profusion of engines with different characteristics. However, task encapsulation, 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 (task encapsulation), 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 are equivalent when integrating new infrastructures (E_4).

The pool architecture is overall the most scalable, which is not surprising since it is designed precisely for scalability. Tight integration is the least scalable and all the other architectures perform the same overall. The global scalability score, however, should not maskthe 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 task encapsulation and nested workflows could well become showstoppersdepending on the type of targeted infrastructure. Non-reliable infrastructures , for example, could hardly cope with workflow engines being wrapped in computing tasks as done in task encapsulation. The availability of multiple engine instances could also become a critical feature for science gateways with important workloads, which would favor task encapsulation 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, task encapsulation 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 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, task encapsulation, 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.

	Tight	Service	Task	Pool	Nested	Import
Integration (global score)	0.00	0.22	0.00	0.44	1.00	0.33
Robustness (global score)	0.14	0.43	0.00	0.71	1.00	0.43
Extensibility (global score)	0.44	0.44	0.00	0.22	1.00	0.22
Scalability (global score)	1.00	0.50	0.50	0.00	0.50	0.50
Specific features (global score)	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 global scores (m' values) of each criterion in Table 2 and the colors are obtained as in Table 2.

4.2. Limitations

A few limitations should be considered when using the results of our evaluation. First, our evaluation methods aimed to provide comparative metrics, however the high-level of abstraction used to derive these metrics hinders the complexity of real systems to some extent.. In particular, the presented architectures are abstract patterns that may be mixed together in actual systems. The distinction between tight integration and service invocation, for instance, may not always be that clear in practice. Service invocation may also be combined with task encapsulation in some cases. However, the criteria discussed in this work would still apply to broadly compare and categorize such cases of hybrid 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, without entering into the details of a particular system, quantification of the robustness or the amount of development associated with each interaction and software component will not be precise.

The particular case of interaction `g` (workflow language conversion) should be further discussedsince this interaction may 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 task encapsulation, 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. Nevertheless, it could be interesting to explore other types of instantiations, in particular nested workflows with task encapsulation.

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 task encapsulation. 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.

Finally, workflow engines are only one of the many aspects involved in the design of a science gateway. Other properties definitely influence the design of a software architecture, for instance collaborative features, data visualization, search, authentication, accounting and so on.

5. Conclusion

We have systematically reviewed architectures used to integrate workflow engines in science gateways. These architectures are described in a system-independent framework suitable for comparison, illustrated on real systems, and evaluated using novel quantitative metrics that allow simple comparison across architectures. We have discussed the pros and cons of all the presented architectures based on these metrics.

To the best of our knowledge, our work is the first of its kind. So far, the literature on science gateways and workflow engines has focused on the description of particular systems, or on the presentation

of a particular architecture. Instead, our analysis abstracts and evaluates architectural patterns independently from any particular system. It provides general insight to integrate science gateways and workflow engines, which we hope will be useful for software architects.

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