# Software architectures to integrate workflow engines in science gateways

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**Abstract**

Science gateways often rely on workflow engines to execute applications on distributed infrastructures. We investigate six software architectures commonly used to integrate workflow engines into 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 conversion*, the engine is integrated through workflow language conversion. We describe and evaluate these architectures with metrics for assessment of integration complexity, robustness, extensibility, scalability and functionality. Tight integration and task encapsulation are the easiest to integrate and the 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 conversion. These results provide insights for science gateway architects and developers.

*Keywords:* Workflow engines, science gateways, software architectures.

## 1. Introduction

Several software architectures can be adopted to integrate workflow engines in the ecosystem of tools and services offered by science gateways, with important consequences for the development effort required and resulting system.

This paper describes, illustrates and compares such architectures, based on system-independent representations of their main components and interactions. It is informed by our experience in the development and sustained operation of the CBRAIN [41], NSG [38, 39] and VIP [17] science gateways during the past 7 years, as well as by lessons learned from several science gateway and workflow projects such as SHIWA[1] and ER-flow[2].

This analysis is intended for experts of science gateway and workflow engine design. It is an abstraction effort to identify and evaluate the fundamental architectural patterns that are encountered while integrating workflow engines and science gateways. In real systems, such patterns sometimes coexist due to the historical and technical context of software projects.

The remainder of this section provides 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 in-

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

teractions between their main software components. We illustrate these architectures on real systems in Section 3. In Section 4, we introduce metrics that measure integration complexity, robustness, extensibility, scalability and functionality. The metrics are specifically designed to measure the ability of the architectures to address workflow-related issues commonly encountered in science gateways. We evaluate the architectures individually in Section 5, and we compare and discuss them in Section 6. Finally, in Section 7, we illustrate how our evaluation framework can be used to help design new systems. Related work is presented in Section 8.

### *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 [16], Hyperflow [5], MOTEUR [18], Pegasus [11, 12], Swift [50], Taverna [32], Triana [43], VisTrails [8], WS-PGRADE [26] and WS-VLAM [47]. Such workflow engines usually describe applications using 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 [22]), PSOM (Pipeline System for Octave and Matlab [6]), PMP (Poor Man's Pipeline [2]), RPPL [51], SPM (Statistical Parametric Mapping [4]) and FSL (FMRIB Software Library [24]) 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 coordinates and 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 engines and domain-specific pipeline systems. Some workflow engines, usually from the e-Science community, 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 [30], the Catania Science Gateway Framework [3] and WS-PGRADE/gUSE [26]. Numerous science gateways were built using such frameworks [25, 3] or as standalone systems [41, 17]. 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 others 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 [28], 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*

An infrastructure consists of the computing and storage resources involved in workflow execution, as well as the software services used to access these resources. The 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, or the presence of a file catalog. In the analysis presented hereafter, 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 presented in Figure 2 using the graphical notations defined in Figure 1. Software components are defined at a granularity such that two components may potentially be operated by different teams on different hardware systems. For instance, the science gateway and infrastructure are usually distinct components. In real systems, software components may exist at a finer granularity, to implement functions such as authentication, data persistence or logging. Such fine-grained components are not covered by our analysis since we focus on the interactions between the science gateway, the infrastructure and the workflow engine.

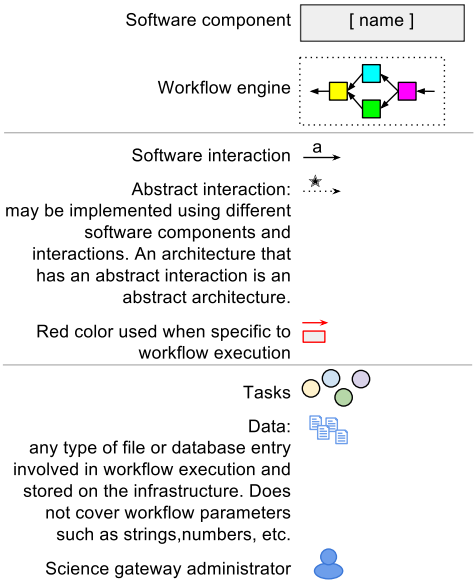



Figure 1: Graphical notations

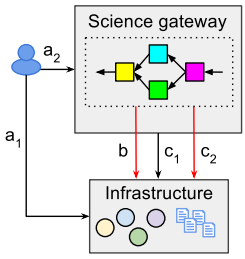
Table 1 summarizes the classification of a few systems by architecture.

### *2.1. Interactions*

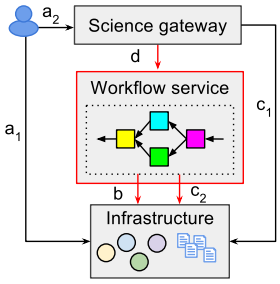
The interactions involved in the architectures are described below and labeled from `a` to `g` as in Figure 2.

`(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: ($\mathtt{a}_1$) the programs used in the workflow are installed on the infrastructure or prepared for on-the-fly deployment, which may require specific privileges; ($\mathtt{a}_2$) 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*.

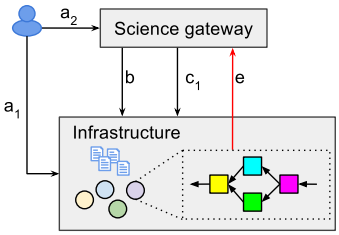
`(b)` Task control: operations to manage tasks on the infrastructure, including authentication, submission, monitoring, termination, deletion, etc. Controlling tasks requires dealing with the heterogeneous batch managers and meta-schedulers that might be available on the infrastructure. When the infrastructure is a grid or a cloud, control may be achieved for instance using libraries that



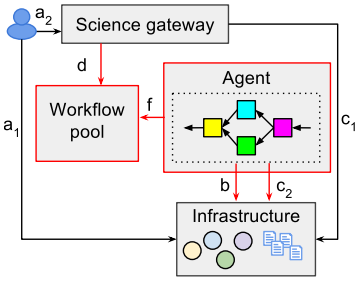

(I) Tight integration



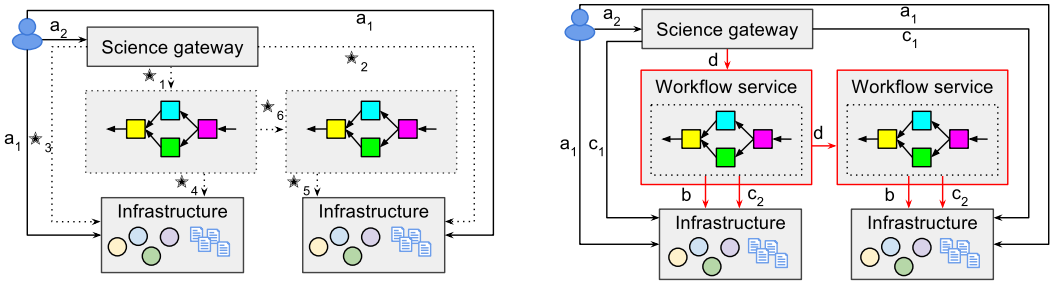

(II) Service invocation



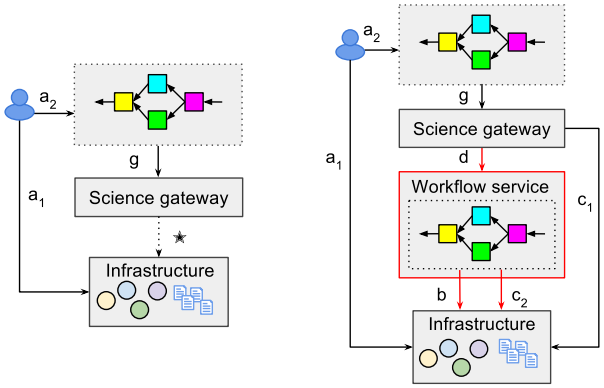

(III) Task encapsulation




(IV) Pool




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




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

Figure 2: Architectures

| Architecture | Systems |
|---|---|
| Tight | Gateways based on the Catania Science Gateway Framework [3], Distributed application runtime environment (DARE [29]), LONI Pipeline Environment [13] |
| Service | Gateways based on Apache Airvata [30], HubZero with Pegasus [31], System in [48], Vine Toolkit [42], Virtual Imaging Platform [17], Gateways based on the WS-PGRADE/gUSE framework [26], GridSFEA [15] |
| Task | CBRAIN and PSOM [19], CBRAIN and FSL |
| Pool | SHIWA pool [37] |
| Nested | SHIWA Simulation Platform (Coarse-Grained Interoperability [44]), HubZero with Pegasus (via hierarchical workflows) [12], Tavaxy [1]. |
| Conversion | SHIWA Simulation Platform (Fine-Grained Interoperability) [35], Tavaxy [1], system in [9]. |

Table 1: Classification of science gateways based on the architecture used to integrate workflow engines.

implement standards such as SAGA (Simple API for Grid Applications [21]), DRMAA (Distributed Resource Management Application API [45]), 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 science gateway ($c_1$), e.g., 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 them. The infrastructure might offer various data storage backends with heterogeneous interfaces. Tools and services such as JSAGA [36] or Data Avenue [23] can be used to homogenize 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 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. 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 [46] and other agent-based computing models.

(g) Workflow conversion: translation from one workflow language into another. This interaction may not be available or possible for every workflow language. It has been developed mostly for translation between well-structured and relatively simple workflow languages such as GWorkflowDL and Scufl [33], and for translation among the 5 workflow systems in the SHIWA project: Askalon, MOTEUR, Taverna, Triana and WS-PGRADE.

### *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[3]. The workflow engine and the science gateway usually share a database where applications, users and other resources are stored. In this model, task

[3]Note that the particular case of portlets can be a bit ambiguous: when portlets are deployed remotely, using protocols such as Web Services for Remote Portlets (WSRP), they become independent software components according to our definition because they could be operated by different teams on different hardware systems. In this case, the system should be classified in the service invocation architecture since the portlets actually become Web Services. The same comment holds for remote object invocation.

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. Tight integration is the model adopted in the Catania Science Gateway Framework [3] (see specific documentation on workflows[4]), in the Distributed application runtime environment (DARE) [29], in Galaxy [20], 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 in some variations of the architecture (not represented in Figure 2) it might as well be delivered by the workflow engine directly to the user.

This architecture is largely adopted in systems such as the Apache Airvata framework [30], GridSFEA [15], Vine Toolkit [42], Virtual Imaging Platform [17], the systems in [48, 39] and the WS-PGRADE/gUSE framework [26]. The integration between the HubZero science gateway and the Pegasus workflow engine performed in [31] 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.).

### *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 submits the sub-tasks to the infrastructure and completely controls them. For instance, it may cancel them when the workflow is canceled. The science gateway may also implement mechanisms to facilitate the handling of task dependencies, for instance lists of tasks that must be completed before a particular task can be executed.

The science gateway also transfers both user and workflow data across the infrastructure, through interaction $c_1$.

### *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 $c_1$, and administrator installs workflows through interaction $a_1$ and $a_2$.

### *2.6. Nested workflows*

See Figure 2(V). In nested workflows (Figure 2(V)-Left), a workflow engine is integrated as a *child* process of a *parent* workflow engine. Parent and child engines might use different languages and might run on different infrastructures. A parent workflow is also a 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 $a_1$ and $a_2$.

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 (Fig-

[4] https://frama.link/jfzgaEbj

ure 2(V)-Right) as this is the most used architecture. We call this instantiation "Service+Service" since both engines are integrated through service invocation. 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 into 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 $c_2$. Science gateway transfers user data to infrastructures using $c_1$.

Nested workflows have long been available in workflow engines, for instance in the Taverna workbench [32]. 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 [44], i.e., to integrate various workflow engines in a consistent platform.

### *2.7. Workflow conversion*

See Figure 2(VI). This is an abstract model instantiated with the service invocation architecture for consistency. Workflow conversion is presented here as a pattern to integrate workflow *engines* in a science gateway, through workflow format conversion from a native format to the science gateway format. Workflow conversion is usually an offline process that is not involved in workflow execution. A few systems have implemented workflow conversion. In the SHIWA Simulation Platform, it is implemented through the IWIR language, which provides a common language for portability across grid workflow systems [35] and allows conversion among $n$ workflow languages using $2n$ interactions instead of $n^2$. Tavaxy [1] enables the import, merging and execution of Taverna [32] and Galaxy [20] 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 conversion from KNIME [7] to WS-PGRADE/gUSE and from Galaxy [20] to WS-PGRADE/gUSE.

## 3. Real systems

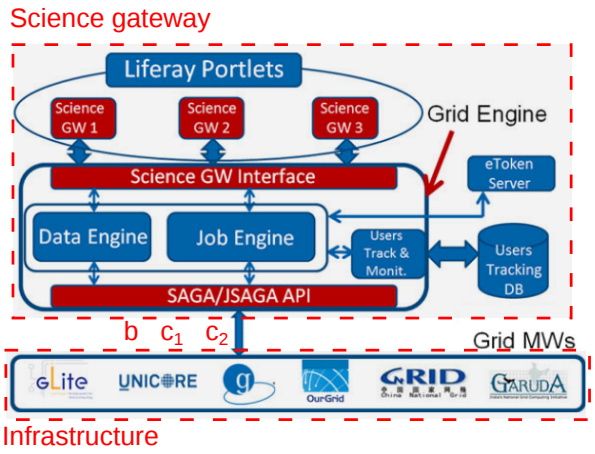



Figure 3: Architecture of the Catania Science Gateway Framework (tight integration). Figure adapted from [3] with permission of the first author (approval still pending).

This section illustrates the architectural patterns on a few real systems, using the original architecture diagrams published by the system developers. To improve readability, we annotated these diagrams with the interactions and components used in Figure 2.

### *3.1. Tight integration*

The architecture of the Catania Science Gateway Framework (CSGF) is shown in Figure 3. In CSGF, workflows are integrated as Liferay portlets, i.e., as part of the science gateway when no specific protocol is used for remote invocation. A specific portlet called `mi-parallel-portlet` allows to create job collections, parametric jobs and split-and-merge types of workflows. The science gateway also includes a set of services to manage data and tasks (jobs) on a wide array of grid middleware systems through the SAGA API.

### *3.2. Service invocation*

Figure 4 shows the architecture of the Virtual Imaging Platform (VIP), where the MOTEUR workflow engine [18] is invoked through a service. The interactions in the VIP architecture map to the ones defined by our framework in a straightforward manner, except for interaction $c_2$ (management of workflow data) which, in VIP, is triggered by the workflow tasks instead of the workflow engine. This does not contradict the service invocation architecture since the tasks are generated by the workflow engine.

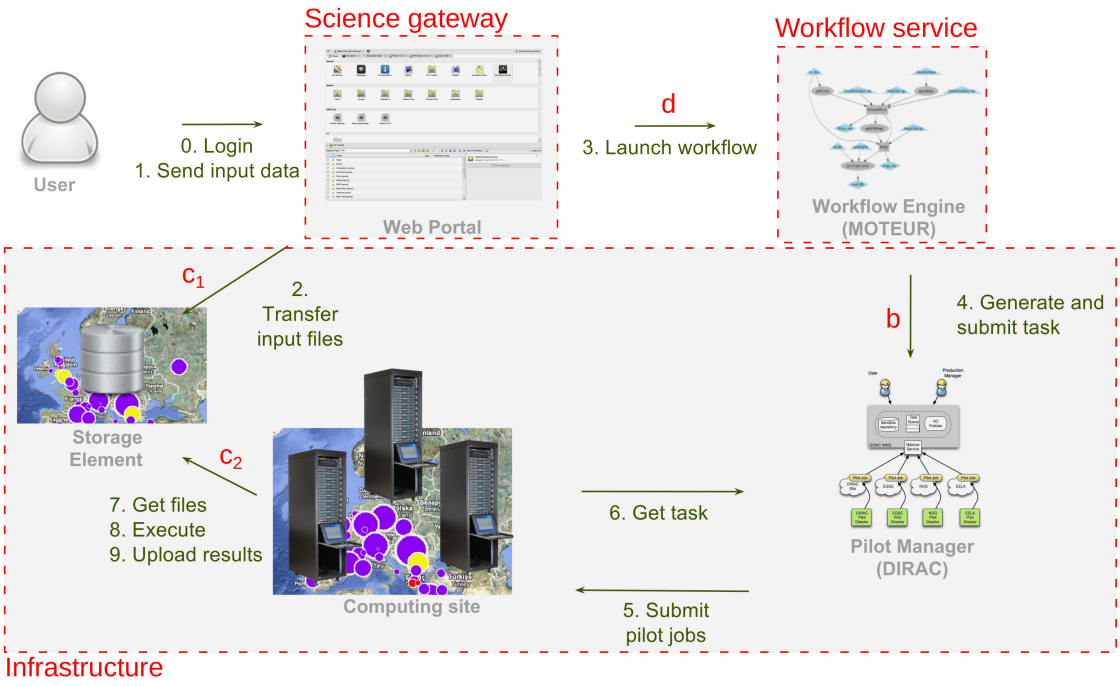



Figure 4: Architecture of the Virtual Imaging Platform (service invocation). Step 3 corresponds to interaction d in Figure 2(II), step 2 corresponds to interaction $c_1$, step 4 maps to interaction b, and steps 7 and 9 map to $c_2$ (in VIP, workflow data transfers are performed by the tasks and embedded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

### *3.3. Task encapsulation*

Task encapsulation is used in the CBRAIN gateway [41] to integrate the FSL toolkit [24] and the PSOM workflow engine [6]. The CBRAIN-FSL integration, shown in Figure 5(I), allows leveraging FSL pipelines written in low-level workflow languages (Linux executables and scripts) that submit tasks uniformly through a specific tool called fsl_sub. The science gateway is actually split in two services, the CBRAIN portal and the CBRAIN execution server deployed on a head node of the infrastructure. The mapping of interactions b, $c_1$ and e to the CBRAIN-FSL interactions is straightforward.

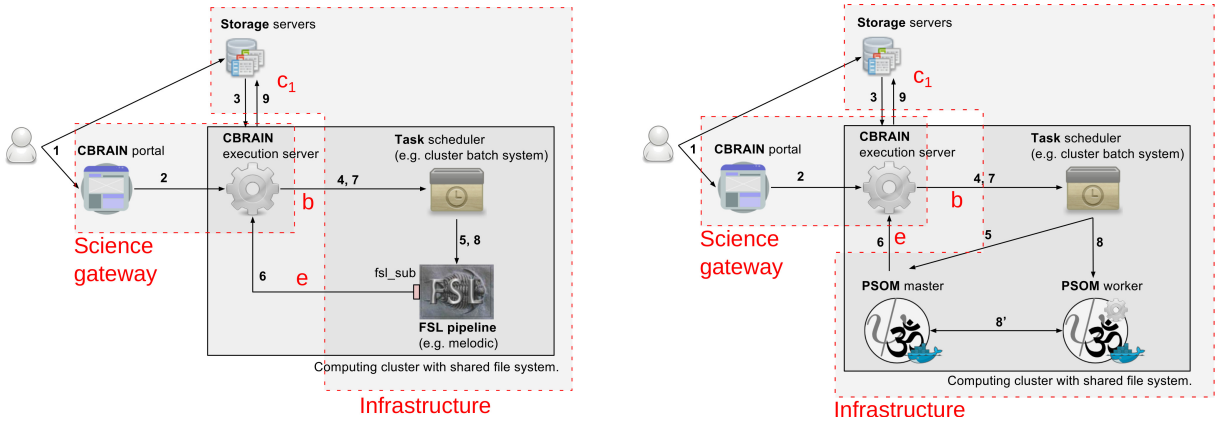
The CBRAIN-PSOM integration [19] is shown in Figure 5(II). The PSOM workflow engine adopts a pilot-job architecture [46] where a master coordinates workflow execution by submitting workers and establishing direct communication channels with them. Note how this peculiar execution model is well supported by task encapsulation.

### *3.4. Pool model*

The pool model was implemented in the SHIWA pool [37] diagrammed in Figure 6, where agents can wrap different types of workflow engines to execute workflows expressed with different languages. The software components map directly to the ones in our architecture, except that the infrastructure is not represented. The interactions described in the SHIWA pool are much finer-grained than in our model, but they can be grouped to match interactions d and f, as explained in the Figure caption.

### *3.5. Nested workflows with service invocation*

Figure 7 shows the architecture used in the SHIWA Simulation Platform for nested workflow execution with service invocation. The parent workflow engine is WS-PGRADE/gUSE, invoked as a service in the Science Gateway (interaction d). Ten different child engines can be used by nested workflows, invoked through the Submission service (interaction d). Each of these engines can submit tasks and transfer data to a distributed computing infrastructure (DCI interactions b and $c_2$). User data interactions ($c_1$) and interactions between the parent engine and the infrastructure (b and $c_2$) are not represented.




(I) CBRAIN-FSL integration. (II) CBRAIN-PSOM integration. Figure adapted from [19].

Figure 5: 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 $c_1$ 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).

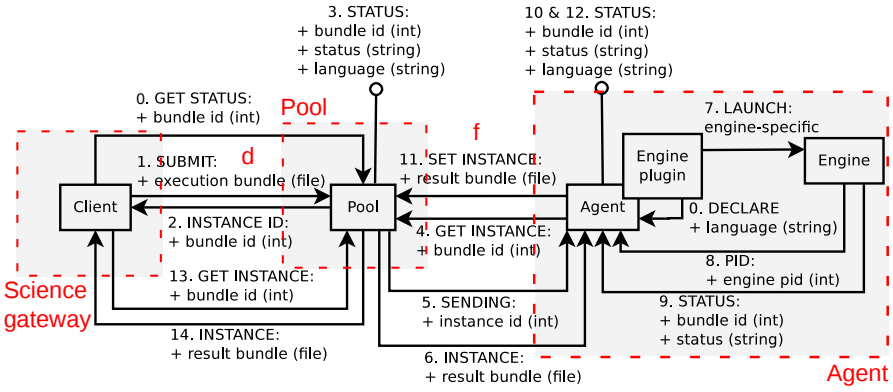



Figure 6: Architecture of the SHIWA pool. Circle-terminated arrows indicate messages that are broadcast to all pool clients. Interaction `d` of Figure 2(IV) is implemented by 3 different calls to the pool: workflow submission (`1` & `2`), workflow status retrieval (`0` & `3`), and workflow retrieval (`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 adapted from [37].

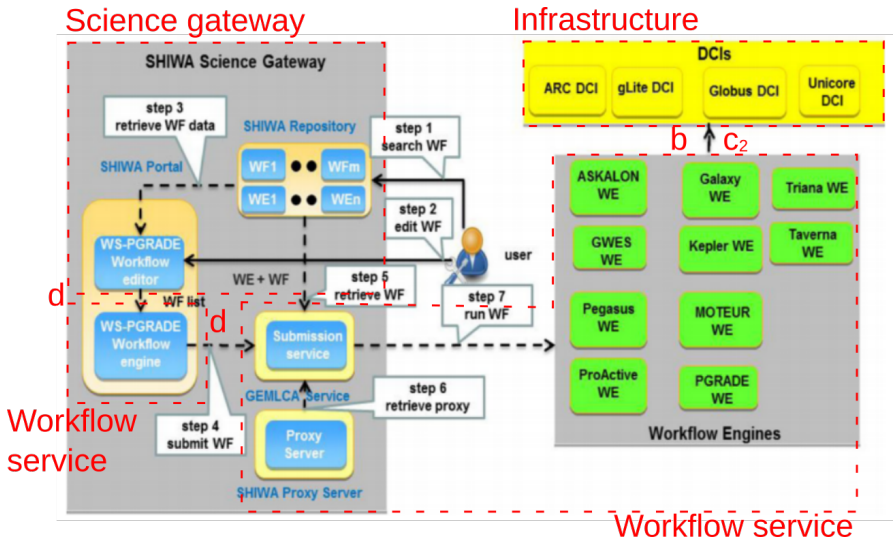



Figure 7: Nested workflow execution through the SHIWA Science Gateway. Figure adapted from [44] with permission of the first author.

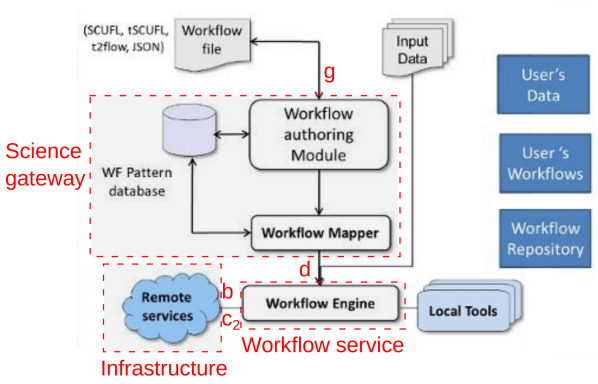



Figure 8: Architecture of Tavaxy (workflow conversion). Figure adapted from [1] with permission of the first author.

### *3.6. Workflow conversion with service invocation*

Figure 8 shows the architecture of Tavaxy where workflows in various formats (tSCUFL, SCUFL, t2flow and JSON) can be imported. As detailed in [1], workflow conversion (interaction g) is implemented through an interactive authoring module where users can check and edit workflow imports, and a mapper module that performs some language substitutions. The workflow engine is a re-engineered version of the Galaxy engine that also includes some components of Taverna.

## 4. Evaluation metrics

The architectures are evaluated in Table 2 using five main criteria: integration complexity, robustness, extensibility, scalability and functionality. Criteria break down into specific metrics where *lower value indicates better performance*. Colors in Table 2 represent normalized scores (see caption). For each criterion, a global score is computed by summing up the individual scores for each metric. We ensure that the different metrics used to calculate the global score for a criterion are comparable, so that they can be combined meaningfully.

The metrics defined hereafter aim at providing a framework to evaluate architectures independently from any particular system, regardless of any technical constraint such as the use of a specific programming language or the internal architecture of the science gateway. The goal is to abstract architectural discussions from the particular technical context of a real system. Some degree of system-specificity can be introduced in the evaluation by assigning weights to interactions and components through a public spreadsheet available at `https://frama.link/LrPRsCQp`[5]. In particular, sheet "Components and interactions" in this spreadsheet contains the weight assigned to components and interactions, which can be used to produce new versions of Table 2 that fit the particular

[5]The spreadsheet may need to be downloaded to be edited.

technical context of a real system. For instance, a high weight could be assigned to the science gateway if its internal architecture is such that it can hardly be extended in practice.

In addition, all the metrics in a criterion contribute equally to the global score used for the criterion. Column B of sheet "Metrics" of the public spreadsheet may be used to assign different weights to each metric to adjust the specific context of a study.

The remainder of this Section defines the metrics in each criterion.

### *4.1. Integration complexity*

Integration complexity is measured through the number of software components and their interactions. It breaks down into the following 2 metrics:

- Total components ($\mathtt{I}_1$): total number of components in the architecture.
- Total interactions ($\mathtt{I}_2$): total number of interactions in the architecture.

One may wonder whether infrastructure should be counted in $\mathtt{I}_1$, since it is usually an external entity that is not developed nor maintained by the groups who integrate workflow engines in science gateway. We support its inclusion here because integrating an infrastructure into the system usually requires some technical effort (e.g., account creation, software installation, APIs, etc.), therefore increasing complexity. The weights given to software components in $\mathtt{I}_1$ and interactions in $\mathtt{I}_2$ can be adjusted in the public spreadsheet to cover the technical peculiarities of a real system.

The two metrics $\mathtt{I}_1$ and $\mathtt{I}_2$ are summed to obtain a global score that measures the total number of software pieces affected by integration.

### *4.2. Robustness of workflow execution*

Robustness of workflow execution measures the likelihood that the workflow execution fails due to errors in the components or in the interactions of 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, in particular in distributed systems where interactions between components involve wide-area network communications between machines that may be operated by different people. More precisely, robustness is determined by the number of software components and interactions represented in red in the architecture diagrams in Figure 2, which are specific to workflow execution. Two metrics are used:

- Specific components ($\mathtt{R}_1$): number of specific components involved in workflow executions. For instance, the workflow service is a specific component because its main objective is to execute workflows. On the contrary, the science gateway is *not* specific to workflow execution since it is used for a variety of other functions such as user authentication, data transfer, etc.
- Specific interactions ($\mathtt{R}_2$): number of specific interactions involved in workflow executions. For instance, the pool-agent interaction (interaction $\mathtt{f}$) is specific to workflow execution while data control (interaction $\mathtt{c}_1$) is *not* because it is used by the science gateway to transfer user data regardless of a particular workflow execution.

$\mathtt{R}_1$ 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. The weights given to software components in $\mathtt{R}_1$ and interactions in $\mathtt{R}_2$ can be adjusted in the public spreadsheet.

### *4.3. Extensibility*

Extensibility measures the difficulty to replace or add elements to the architecture. It is determined by 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 into 4 metrics depending on the type of element (engine, workflow or infrastructure) that has to be added or replaced:

- New engine ($\mathtt{E}_1$): number of interactions or components that need to be modified to integrate a new type of workflow engine in the architecture. Workflow engines belong to different types when they

| | Tight | Service | Task | Pool | Nested Service+Service | Conversion |
|---|---|---|---|---|---|---|
| **Integration 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 | 3 | 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** | **9** | **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** |
| **Functionality** | | | | | | |
| Meta-workflow – $F_1$ | 1 | 1 | 1 | 1 | 0 | 0 |
| Fine-grained debugging – $F_2$ | 0 | 1 | 1 | 1 | 1 | 1 |
| **Total** (missing features) | **1** | **2** | **2** | **2** | **1** | **1** |

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 minimum and maximum values for 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).

cannot be invoked using the same implementation of the interactions.

• Engine version upgrade ($E_2$): number of interactions or components modified 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 can be invoked using the same interaction implementation(s). 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. In practice, $E_2$=0 when the workflow engine is wrapped in a service or in an agent, and $E_2$=1 when it is wrapped in another component.

• New workflow ($E_3$): number of interactions required to integrate a new workflow in the architecture. Adding a new workflow is a very common operation that does not require modifying software components or interactions, assuming that the engine type and version required to execute this workflow are already available. In most cases, adding a new workflow requires only interactions $a_1$ and $a_2$, but g is required as well when workflow conversion is used.

• New infrastructure ($E_4$): number of interactions or components affected for the integration of a new type of infrastructure in the architecture. Adding a new infrastructure typically aims at providing more computing or storage power, enabling access to specific types of resources (e.g., GPUs, clouds), or enforcing execution policies (e.g., constrain data to remain in a particular network domain).

The four metrics are summed to obtain a global score that measures the difficulty to extend the architecture. The weights given to software components and interactions in $E_{1-4}$ can be adjusted in the public spreadsheet. Note that some extensions may affect several metrics in practice. For instance, adding a new type of engine may help integrating

new infrastructures when interactions b and $c_2$ are already present for the new engine and the infrastructure.

### *4.4. Scalability*

Scalability corresponds to the ability of an architecture to cope with high workloads through the following mechanisms: starting multiple engine instances, distributing engines and task scheduling. This is measured by assessing the potential scalability difficulties due to (partial) absence of a given feature in the architecture. Three different features are identified:

• Multiple engine instances ($S_1$): measures the ability for a single gateway instance to use more than one engine instance simultaneously, *each workflow being executed by a single engine instance*. 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 means that adding a new engine instance is inherently supported in the architecture. In this case, elastic engines can be implemented through some kind of auto-scaling mechanism to control the number of engine instances in the architecture. $S_1$=1 means that supporting multiple engine instances requires specific developments in the science gateway or workflow engine. $S_1$=2 means that new engine instances cannot be added.

• Distributed engines ($S_2$): measures the ability 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 means that distributed engines are enabled by the architecture, and $S_2$=1 that they require specific developments in the workflow engine.

• Task scheduling ($S_3$): measures the complexity added by the architecture to implement task scheduling on the infrastructure. Task scheduling typically 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 means that the architecture does not add any additional complexity to the scheduling problem, and $S_3$=1 otherwise.

These three metrics are summed to obtain a global measure of the scalability potential of the architecture.

### *4.5. Functionality*

Functionality includes:

• Meta-workflow ($F_1$): measures the ability to describe meta-workflows from existing workflows. Meta-workflows offer an additional level of flexibility to build workflows from reusable components. $F_1$=0 means that meta-workflows are intrinsically enabled by the architecture (i.e., they can be implemented using the components and interactions already in place), and $F_1$=1 means that they may be implemented with some development effort.

• Fine-grained debugging ($F_2$): availability of fine-grained debugging information about workflow tasks (white box workflow). We call "white box" workflow a workflow where detailed information about individual tasks is available, for instance task statuses, execution logs and resource consumption. On the contrary, a "black box" workflow only displays global information such as the workflow status and the logs of the workflow engine. Fine-grained information about workflow tasks is required to properly troubleshoot workflow executions. It helps workflow users (scientists) identify errors, it allows gateway administrators to troubleshoot executions, and it facilitates debugging by workflow developers. The availability and accuracy of fine-grained debugging information usually depends on the number of software layers between the science gateway and the workflow engine [34]. $F_2$=0 means that the information is directly accessible in the science gateway, $F_2$=1 means that it is obtained through one or more software interactions.

$F_1$ and $F_2$ are summed to obtain a total number of missing features in the architecture.

## 5. Architecture evaluation

The architectures described in Figure 2 are evaluated hereafter with the proposed metrics.

### *5.1. Tight integration*

*Integration complexity.* This architecture does not require any component in addition to the science gateway and infrastructure ($I_1$=2) and 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 modifying 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 complete science gateway ($S_1$=2). Specific IT setups such as load-balancing between web server instances might be used to create new gateway instances, but they would not allow a single gateway instance to use multiple engine instances, which is the point here. Distributed engines are not available by default ($S_2$=1). The architecture does not add any particular complexity to the task scheduling problem since the workflow engine may implement any kind of scheduling policy ($S_3$=0).

*Functionality.* Supporting meta-workflows requires specific developments in the workflow engine or science gateway to allow workflows to execute other workflows ($F_1$=1). For instance, specific Java objects may be implemented in the science gateway framework to execute different types of workflows and link them together. The science gateway can retrieve fine-grained debugging information from the workflow engine directly ($F_2$=0).

### 5.2. 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 ($R_1$=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 implementing the corresponding workflow service, modifying interaction d, and implementing interactions b and $c_2$. However, when a new type of workflow engine is added, it is always possible to reuse either an existing available workflow service or interaction d (when a new workflow service has to be developed). Therefore, $E_1$=3. 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 in $E_2$ 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 $a_1$ 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 in principle supports multiple engine instances through multiple workflow services. Adding a new engine instance, however, requires specific developments in the science gateway ($S_1$=1). Distributing the execution of a single workflow in multiple engines is usually not possible unless the workflow engine has specific abilities ($S_2$=1).

*Functionality.* Meta-workflows require specific developments in the workflow engine or science gateway to allow workflows to execute other workflows. ($F_1$=1). The science gateway needs to invoke interaction d to retrieve fine-grained debugging information from the workflow service ($F_2$=1).

### 5.3. Task encapsulation

*Integration complexity.* Task encapsulation requires only 2 components ($I_1$=2). It involves 5 interactions: $a_1$, $a_2$, b, $c_1$ and e ($I_2$=5).

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

*Extensibility.* Integrating a new type of workflow engine requires developing interaction e and installing the engine on the infrastructure ($E_1$=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 ($E_2$=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 updating interactions $a_1$, b and $c_1$ in the science gateway ($E_4$=3).

*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 task encapsulation. 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 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.

*Functionality.* Task encapsulation does not enable meta-workflows by default ($F_1$=1). Fine-grained debugging information is obtained through interaction b ($F_2$=1).

### 5.4. 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 wrapping the engine into the agent and updating 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, which 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.* By design, new engine instances only require new agents, which can be easily automated ($S_1$=0). Distributed engines are not available by default ($S_2$=1) and the architecture does not add any complexity to the task scheduling problem ($S_3$=0).

*Functionality.* Meta-workflows require specific developments in the workflow engine to enable workflow submission ($F_1$=1). Debugging information is accessed through interactions d and f ($F_2$=1).

### 5.5. 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 necessary ($R_2$=6).

*Extensibility.* Adding a new type of *parent* engine requires implementing the corresponding service, implementing interactions b and $c_2$ in the parent engine, and implementing interaction d in the science gateway and in the parent service ($E_1$=5). Adding a new type of *child* engine only requires implementing the corresponding service, developing interactions b and $c_2$ in the child engine, and implementing 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 reimplementing 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 engine instance requires specific developments 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 can be implemented 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).

*Functionality.* Meta-workflows can be implemented, which is one of the main interest of this architecture ($F_1$=0). Note, however, that the complexity of the architecture increases with the number of engine types involved in meta-workflows: for instance, a meta-workflow with child workflows executed by 2 different types of engines would require an additional workflow service and the corresponding interactions. Debugging information is accessed through interaction d (invoked twice) ($F_2$=1).

### 5.6. Workflow conversion with service invocation

*Integration complexity.* Workflow conversion with service invocation requires the same components as for service invocation ($I_1$=3), and an additional g interaction ($I_1$=7).

*Robustness.* Since workflow conversion is not involved in the execution (it is an offline process), the scores are the same as for 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 re-implementing interaction g in this architecture ($E_1$=1). Note, however, that implementing interaction g can require substantial work depending on the complexity of the workflow 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), the score is the same as for the service architecture ($S_1$=1, $S_2$=1, $S_3$=0).

*Functionality.* Meta-workflows are available after conversion, by connecting workflows in the language used in the science gateway ($F_1$=0). Debugging information is accessible as in the service invocation architecture ($F_2$=1).

## 6. Discussion

### 6.1. Comparison between architectures

Tight integration and task encapsulation are the simplest architectures to integrate, followed by service integration, workflow conversion (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 conversion (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 conversion (with service invocation) perform slightly better when integrating new engines ($E_1$), which makes them useful architectures for science gateways that do not focus on a particular engine. However, task encapsulation, workflow conversion (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 conversion). Workflow conversion 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 conceal 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 task encapsulation and nested workflows may become problematic depending 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 functionality should not be neglected. Nested workflows (with service invocation) and workflow conversion (with service invocation) are the only architectures that intrinsically support meta-workflows. Besides, tight integration is the only architecture that allows fine-grained debugging, which may be critical for efficient user support.

Table 3 provides an overall comparison between architectures, based on the metrics in Table 2. It should be noted that this analysis is only meant for illustration purposes, since it assumes that all criteria have equal weights while real systems would favor some of them. Weights can be adjusted in the public spreadsheet at `https://frama.link/LrPRsCQp` (column B of sheet "Metrics") to produce a custom version of Table 3 if required.

Overall, task encapsulation and workflow conversion perform a bit better than the other architectures and nested workflows stand a bit behind for the reasons mentioned previously.

### *6.2. 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. Nevertheless, the criteria discussed in this work would still be applicable for broadly comparing and categorizing such cases of hybrid architectures.

It should also be noted that all the interactions involved in the architectures were treated equally, whereas 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). 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 hardly be precise. If a particular system is evaluated, the public spreadsheet can be used to adjust the weights given to specific components and interactions based on the technical context.

The particular case of interaction `g` (workflow language conversion) requires particular attention when implementing a real system since 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/Matlab and Python, which are much richer than scientific workflow languages. If not properly validated, workflow language conversion could introduce critical errors impacting the robustness and correctness of the execution.

The abstract nested workflows and workflow conversion 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 have already been implemented in real systems, and because service invocation is largely used. Nevertheless, it could be interesting to explore other types of instantiations.

The particular technical or historical context of a science gateway project may also influence the evaluation of an architecture to integrate workflow engines. For instance, many workflow engines are already available as web services, which tends to favor service invocation (in particular when interactions can be re-purposed), and other science gateways may have strongly tested task and data control features (interactions `b` and $c_1$), which would

| | Tight | Service | Task | Pool | Nested Service+Service | Conversion |
|---|---|---|---|---|---|---|
| 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 | 0.22 | 0.00 | 0.22 | 1.00 | 0.22 |
| Scalability (global score) | 1.00 | 0.50 | 0.50 | 0.00 | 0.50 | 0.50 |
| Functionality (global score) | 0.00 | 1.00 | 1.00 | 1.00 | 0.00 | 0.00 |
| | **1.6** | **2.4** | **1.5** | **2.4** | **3.5** | **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.

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.

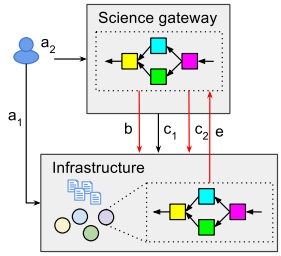



Figure 9: Nested workflow architecture instantiated with tight integration and task encapsulation (Tight+Task).

## 7. Application to systems design

To illustrate how our evaluation framework can be applied to help design new systems, let's consider a hypothetical system where the workflow engine is split in two parts: (1) a high-level part integrated in the science gateway, which submits sub-workflows to the infrastructure; (2) a lower-level part, executed on the infrastructure, which executes the sub-workflows. This scenario came up after the evaluation framework had already been designed.

We model such a system using a nested workflow architecture with a "Tight+Task" instantiation, i.e., the parent engine is tightly integrated in the science gateway and the child engine is integrated through task encapsulation. Figure 9 shows the graphical representation of the system. From this representation we find that the sub-tasks submitted by the child engine through interaction `e` should be handled by the parent engine rather than by the science gateway. Indeed, handling the tasks directly in the science gateway would lead to create a new specific interaction, named, e.g., $\mathtt{b}_1$, while `b` could be reused. We also find that interaction `e` allows running the sub-tasks on the infrastructure(s) supported by the parent engine with no further development effort required in the child engine.

The system evaluation is presented in Table 4. The detailed calculations are available in our public spreadsheet at `https://frama.link/LrPRsCQp`. We conclude that the studied system supports nested workflows with a much better performance than the nested workflow model instantiated with service invocation (evaluated in Table 2): the integration score is improved by a factor of 2, robustness is improved by a factor of 2.6, extensibility is substantially improved, scalability and functionality are not penalized.

## 8. Related work

There is abundant literature describing specific workflow engines and systems; some of the main references are cited in Section 1.1. A few works described the architecture and features of workflow systems at an abstract level. For instance, the early work [49] proposes a generic architecture for grid workflow systems that is based on the workflow reference model defined by the Workflow Management Coalition[6]. Deelman et al. [10] have further characterized the features of workflow systems. These two works, however, do not mention science gateways.

Numerous science gateways have been described, as mentioned in Section 1.2. However, only a few works focused on science gateway architectures.

[6] `http://www.wfmc.org`

| | Nested Tight+Task |
|---|---|
| **Integration complexity** | |
| Total components – $I_1$ | 2 |
| Total interactions – $I_2$ | 6 |
| **Total** | **8** |
| **Robustness** | |
| Specific components – $R_1$ | 0 |
| Specific interactions – $R_2$ | 3 |
| **Total** | **3** |
| **Extensibility** | |
| New engine type – $E_1$ | 3 |
| New engine version – $E_2$ | 1 |
| New workflow – $E_3$ | 2 |
| New infrastructure – $E_4$ | 4 |
| **Total** | **10** |
| **Scalability** | |
| Multiple engine instances – $S_1$ | 1 |
| Distributed engines – $S_2$ | 0 |
| Task scheduling – $S_3$ | 1 |
| **Total** | **2** |
| **Functionality** | |
| Meta-workflow – $F_1$ | 0 |
| Fine-grained debugging – $F_2$ | 1 |
| **Total** | **1** |

Table 4: Evaluation of the nested workflow architecture instantiated with tight integration (parent engine) and task encapsulation (child engine).

Shahand et al. [40] presents the Science Gateway Canvas, which is a business reference model where the most relevant functional components are organized into functional groups. Although workflow management is mentioned as a possible component to coordinate distributed computations in science gateways, the paper does not comment on architecture to achieve this.

Olabarriaga et al. [34] presents a user-centered view of the ecosystem of science gateways with focus on workflow management. Their proposed layered system architecture includes gateway, workflow engine and distributed infrastructure components, similarly to the "service invocation" pattern. However other patterns are not identified.

## 9. Conclusion

We have systematically reviewed architectures used to integrate workflow engines in science gateways. These architectures were 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, and we have shown how our evaluation framework can be leveraged in the design of new systems.

To the best of our knowledge, our work is the first to systematically review and compare software architectures to integrate workflow engines into science gateways. 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, providing general insight about ways to integrate science gateways and workflow engines. These insights will be valuable for software architects when considering alternatives for the architecture and evaluating the impact of their decisions.

## 10. Acknowledgments

We thank the anonymous reviewers for the thorough reviews and useful comments that greatly contributed to improve the quality of this paper. This work has been made possible with the support of the Irving Ludmer Family Foundation and the Ludmer Centre for Neuroinformatics and Mental Health. The integration between PSOM and CBRAIN was supported by a Brain Canada Platform Support Grant, as well as the Canadian Consortium on Neurodegeneration in Aging (CCNA), through a grant from the Canadian Institute of Health Research and funding from several partners. This work is in the scope of the LABEX PRIMES (ANR-11- LABX-0063) of Université de Lyon, within the program "Investissements d'Avenir" (ANR-11-IDEX-0007) operated by the French National Research Agency (ANR). This work also falls into the scope of the scientific topics of the French National Grid Institute (IdG). The VIP team thanks the site administrators of the European Grid Initiative and the GGUS support for their help related to the VIP platform. The CBRAIN team is grateful for the computing cycles, storage, and support obtained from Compute Canada (`https://computecanada.ca`) and platform development program from CANARIE (`http://www.canarie.ca/`). We also acknowledge the Dutch national e-Infrastructure with the support of SURF Cooperative, the Dutch national program COMMIT/ and the High Performance Computing and Networking (HPCN) Fund of the University of Amsterdam for their support to the science gateway actitivies at the AMC. We are also

grateful to the financial support provided by FP7 E-INFRASTRUCTURE program for financial support to SCI-BUS, SHIWA and ER-flow projects.

## References


[1] Mohamed Abouelhoda, Shadi Alaa Issa, and Moustafa Ghanem. Tavaxy: Integrating Taverna and Galaxy workflows with cloud computing support. *BMC Bioinformatics*, 13(1):1–19, 2012.

[2] Y. Ad-Dabbagh, D. Einarson, O. Lyttelton, J.-S. Muehlboeck, K. Mok, O. Ivanov, R.D. Vincent, C. Lepage, J. Lerch, E. Fombonne, and A.C Evans. The CIVET Image-Processing Environment: A Fully Automated Comprehensive Pipeline for Anatomical Neuroimaging Research. In *Proceedings of the 12th Annual Meeting of the Organization for Human Brain Mapping*, 2006.

[3] Valeria Ardizzone, Roberto Barbera, Antonio Calanducci, Marco Fargetta, E Ingrà, Ivan Porro, Giuseppe La Rocca, Salvatore Monforte, R Ricceri, Riccardo Rotondo, et al. The DECIDE science gateway. *Journal of Grid Computing*, 10(4):689–707, 2012.

[4] John Ashburner. SPM: A history. *NeuroImage*, 62(2):791 – 800, 2012.

[5] Bartosz Balis. Hyperflow: A model of computation, programming approach and enactment engine for complex distributed workflows. *Future Generation Computer Systems*, 55:147–162, 2016.

[6] Pierre Bellec, Sébastien Lavoie-Courchesne, Phil Dickinson, Jason Lerch, Alex Zijdenbos, and Alan C Evans. The Pipeline System for Octave and Matlab (PSOM): a lightweight scripting framework and execution engine for scientific workflows. *Frontiers in neuroinformatics*, 6(7), 2012.

[7] Michael R. Berthold, Nicolas Cebron, Fabian Dill, Thomas R. Gabriel, Tobias Kötter, Thorsten Meinl, Peter Ohl, Christoph Sieb, Kilian Thiel, and Bernd Wiswedel. *Data Analysis, Machine Learning and Applications: Proceedings of the 31st Annual Conference of the Gesellschaft für Klassifikation e.V., Albert-Ludwigs-Universität Freiburg, March 7–9, 2007*, chapter KNIME: The Konstanz Information Miner, pages 319–326. Springer Berlin Heidelberg, Berlin, Heidelberg, 2008.

[8] S. P. Callahan, J. Freire, J. Freire, E. Santos, C. E. Scheidegger, C. T. Silva, and Huy T. Vo. Managing the Evolution of Dataflows with VisTrails. In *22nd International Conference on Data Engineering Workshops (ICDEW'06)*, pages 71–71, 2006.

[9] Luis de la Garza, Johannes Veit, Andras Szolek, Marc Röttig, Stephan Aiche, Sandra Gesing, Knut Reinert, and Oliver Kohlbacher. From the desktop to the grid: scalable bioinformatics via workflow conversion. *BMC Bioinformatics*, 17(1):1–12, 2016.

[10] Ewa Deelman, Dennis Gannon, Matthew Shields, and Ian Taylor. Workflows and e-Science: An overview of workflow system features and capabilities. *Future Generation Computer Systems*, 25(5):528–540, 2009.

[11] Ewa Deelman, Gurmeet Singh, Mei-Hui Su, James Blythe, Yolanda Gil, Carl Kesselman, Gaurang Mehta, Karan Vahi, G Bruce Berriman, John Good, et al. Pegasus: A framework for mapping complex scientific workflows onto distributed systems. *Scientific Programming*, 13(3):219–237, 2005.

[12] Ewa Deelman, Karan Vahi, Gideon Juve, Mats Rynge, Scott Callaghan, Philip J. Maechling, Rajiv Mayani, Weiwei Chen, Rafael Ferreira da Silva, Miron Livny, and Kent Wenger. Pegasus, a workflow management system for science automation. *Future Generation Computer Systems*, 46:17 – 35, 2015.

[13] Ivo D Dinov, John D Van Horn, Kamen M Lozev, Rico Magsipoc, Petros Petrosyan, Zhizhong Liu, Allan MacKenzie-Graham, Paul Eggert, Douglas S Parker, and Arthur W Toga. Efficient, distributed and interactive neuroimaging data analysis using the LONI pipeline. *Frontiers in Neuroinformatics*, 3(22), 2009.

[14] Andy Edmonds, Thijs Metsch, Alexander Papaspyrou, and Alexis Richardson. Toward an open cloud standard. *Internet Computing, IEEE*, 16(4):15–25, 2012.

[15] Ekaterina Elts, Ioan Lucian Muntean, and Hans-Joachim Bungartz. *High Performance Computing in Science and Engineering, Garching/Munich 2009: Transactions of the Fourth Joint HLRB and KONWIHR Review and Results Workshop, Dec. 8-9, 2009, Leibniz Supercomputing Centre, Garching/Munich, Germany*, chapter Grid Workflows for Molecular Simulations in Chemical Industry, pages 651–662. Springer Berlin Heidelberg, 2010.

[16] Thomas Fahringer, Radu Prodan, Rubing Duan, Francesco Nerieri, Stefan Podlipnig, Jun Qin, Mumtaz Siddiqui, Hong-Linh Truong, Alex Villazon, and Marek Wieczorek. Askalon: A grid application development and computing environment. In *Proceedings of the 6th IEEE/ACM International Workshop on Grid Computing*, pages 122–131. IEEE Computer Society, 2005.

[17] T. Glatard, C. Lartizien, B. Gibaud, R. Ferreira da Silva, G. Forestier, F. Cervenansky, M. Alessandrini, H. Benoit-Cattin, O. Bernard, S. Camarasu-Pop, N. Cerezo, P. Clarysse, A. Gaignard, P. Hugonnard, H. Liebgott, S. Marache, A. Marion, J. Montagnat, J. Tabary, and D. Friboulet. A virtual imaging platform for multi-modality medical image simulation. *IEEE Transactions on Medical Imaging*, 32(1):110–118, 2013.

[18] T. Glatard, J. Montagnat, D. Lingrand, and X. Pennec. Flexible and efficient workflow deployment of data-intensive applications on grids with MOTEUR. *Journal of High Performance Computing and Applications*, 22(3):347–360, 2008.

[19] T. Glatard, P.O. Quirion, R. Adalat, N. Beck, R. Bernard, B.L. Caron, Q. Nguyen, P. Rioux, M-E. Rousseau, A.C. Evans, and P. Bellec. Integration between PSOM and CBRAIN for distributed execution of neuroimaging pipelines. In *Meeting of the Organization for Human Brain Mapping, Geneva, Switzerland*, 2016.

[20] Jeremy Goecks, Anton Nekrutenko, James Taylor, et al. Galaxy: a comprehensive approach for supporting accessible, reproducible, and transparent computational research in the life sciences. *Genome Biol*, 11(8):R86, 2010.

[21] Tom Goodale, Shantenu Jha, Hartmut Kaiser, Thilo Kielmann, Pascal Kleijer, Gregor Von Laszewski, Craig Lee, Andre Merzky, Hrabri Rajic, and John Shalf. SAGA: A Simple API for Grid Applications. High-level application programming on the Grid. *Computational Methods in Science and Technology*, 12(1):7–20, 2006.

[22] Krzysztof Gorgolewski, Christopher D Burns, Cindee Madison, Dav Clark, Yaroslav O Halchenko, Michael L Waskom, and Satrajit S Ghosh. Nipype: a flexible, lightweight and extensible neuroimaging data process-

ing framework in Python. *Frontiers in Neuroinformatics*, 5(3), 2011.

[23] Ákos Hajnal, Zoltán Farkas, and Péter Kacsuk. Data avenue: remote storage resource management in WS-PGRADE/gUSE. In *6th International Workshop on Science Gateways (IWSG)*, pages 1–5. IEEE, 2014.

[24] Mark Jenkinson, Christian F. Beckmann, Timothy E.J. Behrens, Mark W. Woolrich, and Stephen M. Smith. FSL. *NeuroImage*, 62(2):782 – 790, 2012.

[25] Peter Kacsuk. *Science Gateways for Distributed Computing Infrastructures*. Springer, 2014.

[26] Peter Kacsuk, Zoltan Farkas, Miklos Kozlovszky, Gabor Hermann, Akos Balasko, Krisztian Karoczkai, and Istvan Marton. WS-PGRADE/gUSE Generic DCI Gateway Framework for a Large Variety of User Communities. *Journal of Grid Computing*, 10(4):601–630, 2012.

[27] Jens Kruger, Richard Grunzke, Sandra Gesing, Sebastian Breuers, André Brinkmann, Luis de la Garza, Oliver Kohlbacher, Martin Kruse, Wolfgang E Nagel, Lars Packschies, et al. The MoSGrid science gateway–a complete solution for molecular simulations. *Journal of Chemical Theory and Computation*, 10(6):2232–2245, 2014.

[28] Tania Lorido-Botrán, José Miguel-Alonso, and Jose Antonio Lozano. Auto-scaling techniques for elastic applications in cloud environments. *Department of Computer Architecture and Technology, University of Basque Country, Tech. Rep. EHU-KAT-IK-09*, 12, 2012.

[29] Sharath Maddineni, Joohyun Kim, Yaakoub El-Khamra, and Shantenu Jha. Distributed application runtime environment (DARE): a standards-based middleware framework for science-gateways. *Journal of Grid Computing*, 10(4):647–664, 2012.

[30] Suresh Marru, Lahiru Gunathilake, Chathura Herath, Patanachai Tangchaisin, Marlon Pierce, Chris Mattmann, Raminder Singh, Thilina Gunarathne, Eran Chinthaka, Ross Gardler, et al. Apache Airavata: a framework for distributed applications and computational workflows. In *Proceedings of the 2011 ACM workshop on Gateway computing environments*, pages 21–28. ACM, 2011.

[31] Michael McLennan, Steven Clark, Ewa Deelman, Mats Rynge, Karan Vahi, Frank McKenna, Derrick Kearney, and Carol Song. HUBzero and Pegasus: integrating scientific workflows into science gateways. *Concurrency and Computation: Practice and Experience*, 27(2):328–343, 2015.

[32] Tom Oinn, Matthew Addis, Justin Ferris, Darren Marvin, Martin Senger, Mark Greenwood, Tim Carver, Kevin Glover, Matthew R Pocock, Anil Wipat, et al. Taverna: a tool for the composition and enactment of bioinformatics workflows. *Bioinformatics*, 20(17):3045–3054, 2004.

[33] S. Olabarriaga, T. Glatard, A. Hoheisel, A. Nederveen, and D. Krefting. Crossing HealthGrid Borders: Early Results in Medical Imaging. In *HealthGrid'09*, pages 62–71, Berlin, jun 2009.

[34] Silvia Olabarriaga, Gabrielle Pierantoni, Giuliano Taffoni, Eva Sciacca, Mahdi Jaghoori, Vladimir Korkhov, Giuliano Castelli, Claudio Vuerli, Ugo Becciani, Eoin Carley, et al. Scientific workflow management–for whom? In *e-Science (e-Science), 2014 IEEE 10th International Conference on*, pages 298–305. IEEE, 2014.

[35] Kassian Plankensteiner, Radu Prodan, Matthias Janetschek, Thomas Fahringer, Johan Montagnat, David Rogers, Ian Harvey, Ian Taylor, Ákos Balaskó, and Péter Kacsuk. Fine-Grain Interoperability of Scientific Workflows in Distributed Computing Infrastructures. *Journal of Grid Computing*, 11(3):429–456, September 2013.

[36] Sylvain Reynaud. Uniform access to heterogeneous grid infrastructures with JSAGA. In *Production grids in Asia*, pages 185–196. Springer, 2010.

[37] D. Rogers, I. Harvey, T.T. Huu, K. Evans, T. Glatard, I. Kallel, I. Taylor, J. Montagnat, A. Jones, and A. Harrison. Bundle and pool architecture for multi-language, robust, scalable workflow executions. *Journal of Grid Computing*, 11(3):457–480, September 2013 2013.

[38] Shayan Shahand, Ammar Benabdelkader, Mohammad Mahdi Jaghoori, Mostapha al Mourabit, Jordi Huguet, Matthan WA Caan, Antoine HC Kampen, and Sílvia D Olabarriaga. A data-centric neuroscience gateway: design, implementation, and experiences. *Concurrency and Computation: Practice and Experience*, 27(2):489–506, 2015.

[39] Shayan Shahand, Mark Santcroos, Antoine H.C. vanKampen, and Sílvia Olabarriaga. A grid-enabled gateway for biomedical data analysis. *Journal of Grid Computing*, 10(4):725–742, 2012.

[40] Shayan Shahand, Antoine H. C. van Kampen, and Sílvia D. Olabarriaga. Science Gateway Canvas: A business reference model for Science Gateways. In *Proceedings of the Science of Cyberinfrastructure: Research, Experience, Applications and Models*, SCREAM'15, Portland, OR, USA, 2015.

[41] Tarek Sherif, Pierre Rioux, Marc-Etienne Rousseau, Nicolas Kassis, Natacha Beck, Reza Adalat, Samir Das, Tristan Glatard, and Alan C Evans. CBRAIN: a web-based, distributed computing platform for collaborative neuroimaging research. *Frontiers in Neuroinformatics*, 8(54), 2014.

[42] Dawid Szejnfeld, Piotr Dziubecki, Piotr Kopta, Michal Krysinski, Tomasz Kuczynski, Krzysztof Kurowski, Bogdan Ludwiczak, Tomasz Piontek, Dominik Tarnawczyk, Malgorzata Wolniewicz, Piotr Domagalski, Jaroslaw Nabrzyski, and Krzysztof Witkowski. Vine Toolkit - Towards portal based production solutions for scientific and engineering communities with grid-enabled resources support. *Scalable Computing: Practice and Experience*, 11(2), 2010.

[43] Ian Taylor, Matthew Shields, Ian Wang, and Andrew Harrison. The Triana workflow environment: Architecture and applications. In *Workflows for e-Science*, pages 320–339. Springer, 2007.

[44] Gabor Terstyanszky, Tamas Kukla, Tamas Kiss, Peter Kacsuk, Ákos Balaskó, and Zoltan Farkas. Enabling scientific workflow sharing through coarse-grained interoperability. *Future Generation Computer Systems*, 37:46–59, 2014.

[45] Peter Tröger, Roger Brobst, Daniel Gruber, Mariusz Mamonski, and Daniel Templeton. Distributed resource management application API Version 2 (DRMAA). In *Technical report, Open Grid Forum, January 2012. Also available online:* `http://www.ogf.org/documents/GFD.194.pdf`, 2012.

[46] Matteo Turilli, Mark Santcroos, and Shantenu Jha. A comprehensive perspective on the pilot-job abstraction. *arXiv preprint arXiv:1508.04180*, 2015.

[47] V. Korkhov, D. Vasyunin, A. Wibisono, V. Guevara-

Masis, A.Belloum, C. de Laat, P. Adriaans, L.O. Hertzberger. WS-VLAM: Towards a Scalable Workflow System on the Grid. In *Proceedings of the 2nd workshop on Workflows in Support of Large-Scale Science (WORKS07), 16th IEEE International Symposium on High Performance Distributed Computing*, pages 63–68, 2007.

[48] Wenjun Wu, Thomas Uram, Michael Wilde, Mark Hereld, and Michael E Papka. Accelerating science gateway development with Web 2.0 and Swift. In *Proceedings of the 2010 TeraGrid Conference*, page 23. ACM, 2010.

[49] J. Yu and R. Buyya. A taxonomy of workflow management systems for grid computing. *Journal of Grid Computing*, 3(3-4):171–200, 2005.

[50] Yong Zhao, Mihael Hategan, Ben Clifford, Ian Foster, Gregor Von Laszewski, Veronika Nefedova, Ioan Raicu, Tiberiu Stef-Praun, and Michael Wilde. Swift: Fast, reliable, loosely coupled parallel computation. In *IEEE Congress on Services*, pages 199–206, 2007.

[51] A. P. Zijdenbos, R. Forghani, and A. C. Evans. Automatic "pipeline" analysis of 3-D MRI data for clinical trials: application to multiple sclerosis. *IEEE Transactions on Medical Imaging*, 21(10):1280–1291, Oct 2002.