Designing Workflow Systems Using Building Blocks

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ABSTRACT

We suggest there is a need for a fresh perspective on the design and development of workflow systems and argue for a building blocks approach. We outline a description of this approach and define the properties of software building blocks. We discuss RADICAL-Cybertools as one implementation of the building blocks concept, showing how they have been designed and developed in accordance with this approach. Four case studies are presented, covering a dozen science problems. We discuss how RADICAL-Cybertools have been used to develop new workflow systems capabilities and integrated to enhance existing ones, illustrating the applicability and potential of software building blocks. In doing so, we have begun an investigation of an alternative approach to thinking about the design and implementation of workflow systems.

CCS Concepts

• Software and its engineering → Client-server architectures;

Keywords

Scientific Workflows, Building Blocks, Distributed Systems

1. INTRODUCTION

Sophisticated and scalable workflows have come to epitomize advances in computational science, especially for “big science” projects, such as those in high-energy physics or astronomy. Workflows are also becoming more pervasive across application types, scales and communities.

Interestingly, many commonly used workflow systems in high-performance and distributed computing such as Kepler [1], Pegasus [2], and Swift [3] emerged from an era when the software landscape supporting distributed computing was fragile, missing features and services. Not surprisingly, these initial and many subsequent workflow systems, had a monolithic design that included the end-to-end capabilities needed to execute workflows on heterogeneous and distributed cyberinfrastructures.

In spite of the many successes of workflow systems, there is a perceived barrier-to-entry and limited flexibility. There continues to be an absence of a reasoning framework for end-users to determine which systems to use, when and why. For example, such a lack of clarity and guidance was cited as the single most pressing barrier to workflow adoption by participants of a recent Blue Waters Workflows Workshop. These issues in part are a consequence of the lack of a structured approach to system design and of an unsustainable fragmented ecosystem comprised of systems that often need to establish exclusivity (i.e., “vendor lock-in”) or by preserving “domains of influence”.

Without negating monolithic workflow systems where the socio-technical needs warrant them and make their use meaningful, a valid question is whether it is possible to construct workflow systems or extend the available ones avoiding some of the aforementioned shortcomings. This question is set against the increasing richness of workflow-based applications and consequent demands on workflow systems. Is it possible to design these systems to provide greater flexibility and sharing of features while not constraining functionality, performance, or sustainability?

An important but often overlooked fact is that the majority of scientific workflows don’t use existing workflow systems. The reasons are varied and are not just limited to the proverbial “last mile customization” challenge of workflows. A corollary to the above observation is that there is a need for a sustainable ecosystem of software components from which tailored workflow systems can be composed, as opposed to having to fit workflows to pre-existing solutions.

Thus, the challenge is to support the development and composition of workflow systems that can be responsive to the wide range of workflow requirements. This challenge supersedes the need to develop a software to substitute all other workflow systems, or to interoperate with all of them.

Several additional factors motivate a discussion of alternative approaches to the design and engineering of workflow systems. These systems need to be better prepared for new application scenarios (e.g., integration of large-scale experiments, instruments and observation devices with high-performance computing), scale (e.g., exascale high-performance computing), while improving our ability to create lower-cost and sustainable solutions. Furthermore, the variety and importance of applications with a large number of possibly concurrent simulations are growing while, at the same time, the software platforms and services available...
This paper makes the case for taking a fresh perspective to the design, development and integration of workflow systems by means of a building blocks approach. In the next section we describe this approach and its four design principles of self-sufficiency, interoperability, composability, and extensibility. We postulate the building blocks approach overcomes the limited flexibility of monolithic workflow systems without the significant burden typically associated with integrating disparate software systems. We also argue that the building block approach is a better fit for the typical academic development and economic model, and that developing software building blocks complements the existing systems by helping to avoid software duplication, resource starvation and lack of functionalities.

Section 3 discusses how we used the building blocks approach to design and develop RADICAL-Cybertools. These are a set of software modules that can be used independently, composed into a single system, or integrated into existing systems to extend their functionalities. We introduce a four-layered view of high-performance and distributed systems and we describe how each software module implements distinctive functionalities for each layer.

Section 4 discusses four case studies of employing RADICAL-Cybertools as building blocks to develop or integrate workflow systems. The first study describes the creation of domain-specific workflow systems tailored to the biomolecular and seismology domains. The other three studies illustrate how the functionalities of mainstream workflow systems can be extended by integrating RADICAL-Cybertools. The case studies cover different types of applications, ranging from distributed high-throughput analysis jobs on single nodes (PanDA), to multiple simulations (SeisFlows, HTBAC, FireWorks) to adaptive workflows of biomolecular simulations (RepEx, ExTASY).

We conclude with a discussion of the practical impact of the case studies as well as the lessons learnt by testing the validity and feasibility of the building blocks approach. We highlight the benefits of implementing new capabilities into existing workflow systems by integrating the RADICAL-Cybertools. We also outline the limitations of our contributions as well as some open questions.

Terminology: The term ‘workflow’ is often overloaded in literature and used for a wide variety of scenarios in the computational science discourse. Sometimes, the term workflow is used to describe the computational process associated with an application; sometimes to indicate the application itself. To add to the confusion, ‘workflows’ are sometimes also used as a reference to the task graph (i.e., tasks and their relationships) representing the application. Even when there is clarity on what a workflow describes, a complicating factor is that there are multiple distinct specifications of the same workflow.

Another common source of confusion is the conflation between similar but distinct concepts, such as those of workflow and workload. In this paper, we adopt the following definitions: A multi-task application can be represented as a workflow, i.e., a set of tasks with dependencies that determine the order of their execution. Subsets of these tasks can be workloads, i.e., tasks whose dependencies have been satisfied at a particular point in time and that may be executed concurrently. In this way, workflow provides a complete description of the execution process while workload identifies the entity that is executed. We maintain that these characteristics are independent of the scale of the application, the number of users (or developers) of the workflow or type of workflow (compute or data-intensive). As such, Workflow systems and Workload systems control different entities.

Although the focus of this paper is on using the building blocks approach to design, develop, and integrate workflow systems, the approach we propose is equally applicable to workload management systems, prominent examples of which are PanDA [4], glideinWMS [5] or DIRAC [6].

2. BUILDING BLOCK APPROACH

The building block approach is related to the methods presented in Ref. [7][8][9]. In this paper, we apply this approach to the design of middleware for the execution of scientific workflows. In our adaptation, the building block approach is used to describe the architectural design of workflow systems and is based on four design principles: self-sufficiency, interoperability, composability, and extensibility.

A software building block is self-sufficient when its design does not depend on the specificity of other building blocks; interoperable when it can be used in diverse system architectures without semantic modifications; composable when its interfaces enable communication and coordination with other building blocks; and extensible when the building’s block functionalities and entities can be extended to support new requirements or capabilities.

For example, a system component designed to handle only a single type of workflow does not satisfy the principle of self-sufficiency. Analogously, a system capable of managing multiple types of workflows but only when expressed in a specific representation does not satisfy the principle of interoperability. Software systems designed for unidirectional communication or without the capability to enable coordination cannot be composed so as to form a distributed system with end-to-end capabilities. Finally, systems that cannot be extended cannot guarantee sustained interoperability and composability.

Each building block has a set of entities and a set of functionalities that operate on these entities. Architecturally, a building block designed in accordance with the method we propose has: (i) two well-defined and stable interfaces, one for input and one for output; (ii) one or more conversion layers capable of translating across diverse representations of the same type of entity; (iii) one or more modules implementing the functionalities to operate on these entities. While this architecture is relatively common, it has been seldom applied to the design of middleware systems for the execution of scientific workflows.

Self-sufficiency and interoperability depend upon the choice of both entities and functionalities. Entities have to be general enough so that specific instances of that type of entity can be reduced to a unique abstract representation. Accordingly, the scope of the functionalities of each building block has to be limited exclusively to its entities. In this way, interfaces can be designed to receive and send diverse codifications of the same type of entity, while functionalities can be codified to translate consistently those representation into a generic set of properties, and operate on them.

Composibility depends on whether the interfaces of each building block enables communication and coordination. Blocks communicate information about the states, events
3. RADICAL CYBERTOOLS

RADICAL-Cybertools are software modules designed and implemented in accordance with the building block approach described in Section 2. Each module has been designed independent from one another and with well-defined functionalities and entities. Fig. 1 shows four RADICAL-Cybertools modules alongside their inter-relationships: RADICAL-SAGA [12], RADICAL-Pilot [13], RADICAL-WLMS [14], and RADICAL Ensemble-Toolkit hereafter simply referred as EnTK [15].

We briefly discuss a four-layered view of high-performance and distributed systems as depicted in Fig. 1 to appreciate the design of individual RADICAL-Cybertools as well as their overall organization.

Each layer has a well-defined functionality and an associated “entity”. The entities start from workflows (or applications) at the top layer and resource specific jobs at the bottom layer, with intervening transitional entities of workloads and tasks. The diagram of Fig. 2 provides a reference example for transitions between these entities across layers that is independent of the specifics of workload and resources.

Workflow and Application Description Level (L4): Provides an expressive yet flexible way to capture the requirements and semantics of the applications and workflows.

Workload Management (WLM) Level (L3): Applications devoid of semantic context are expressed as workloads, which are a set of tasks whose relationships and dependencies are expressed as a computational graph. The Workload Management layer is responsible for: (i) the selection and configuration of available resources for the given workload; (ii) partitioning the workload over the selection of suitable resource; (iii) binding of constituent tasks to resources; and (iv) the management and coordination of these three functional aspects.

Task Execution Runtime Level (L2): L3 delivers tasks to L2 which is responsible for their effective and efficient execution on the selected resources. L2 is a passive recipient of tasks from L3 but includes an active module that maps the tasks onto a scheduling overlay comprised of the chosen

![Figure 1: End to end composition of RADICAL-Cybertools. Numbered levels on the left; names of entities on the right. Solid colored lines indicate composition between workflows/applications and RADICAL-Cybertools; dashed lines composition among RADICAL-Cybertools. Blue, orange, and green lines indicate how tools, mini-apps [16] [17], workflow systems and domain-specific workflows (DSW) are executed via alternative compositions of RADICAL-Cybertools.](image-url)
computing resources.

Resource Layer (L1): The resources used to execute tasks are characterized by their capabilities, availability and interfaces. At L1, all tasks have been wrapped up as resource specific jobs; while the semantic inconsistency in the capabilities of resources remains, each job can be submitted to diverse resources thanks to advances in syntactically uniform resource access layers.

We now discuss the four RADICAL-Cybertools and how they conform to the principles of self-sufficiency, interoperability, composability and extensibility.

RADICAL-SAGA exposes a homogeneous programming interface to the queuing systems of HPC, HTC, and cloud resources. SAGA—an OGF standard [12]—abstracts away the specificity of each queue system, offering a consistent representation of jobs and of the capabilities required to submit them to the resources. The design of RADICAL-SAGA is based on the job entity and the scope of its functionalities is limited to job submission and jobs’ requirements handling (self-sufficiency). Both entities and functionalities can be extended to support, for example, new queue systems or new type of jobs (extensibility). The SAGA API resolves the differences of each queue system into a general and sufficient representation (interoporability), exposing a stable set of capabilities to both users and/or other software elements (composability).

RADICAL-Pilot is a pilot system implemented in accordance with the pilot model described in Ref. [13][19]. RADICAL-Pilot exposes an API to enable the acquisition of resource placeholders on which to schedule workloads for execution. This API is implemented both as a library and as a RESTful service. The design of RADICAL-Pilot includes pilot, and compute and data unit as entities. Capabilities are made available to describe, schedule, manage and execute entities. Pilots, units and their functionalities abstract the specificities of diverse type of resources, enabling the use of pilots on single and multiple HPC, HTC, and cloud resources. A pilot can span single or multiple compute nodes, resource pools, or virtual machines. Units of various size and duration can be executed, supporting MPI and non-MPI executables, with a wide range of execution environment requirements.

The design of RADICAL-Pilot [13][20] is: self-sufficient due to the generality and well-defined scope of its entities and functionalities; interoperable in terms of type of workload, resource, and execution requirements; and extensible as new properties can be added to the pilot and unit description, and more capabilities can be implemented without altering its design. Currently, composability is partially designed and implemented: while the PILOT-API can be used by both users and other systems to describe one or more generic workloads for execution, RADICAL-Pilot interfaces to resources requires SAGA. A system based on dedicated resource connectors, including but not limited to SAGA, is currently being designed.

The design of RADICAL-WLMS is also an ongoing project. Developed as a prototype to study and test a general model of workload management, RADICAL-WLMS is being developed to be agnostic towards the modalities used by users or systems to provide workloads descriptions. RADICAL-WLMS integrates information about the workload requirements and the resource capabilities, explicitly separating the planning and management of each workload execution. RADICAL-WLMS uses an abstraction called “execution strategy” for the homogeneous specification of alternative execution plans, and an execution manager to enact each plan. Workloads are executed over one or more pilots, with number of cores and duration tailored to the requirements of the workload. Pilots are concurrently scheduled on one or more resources, and units are scheduled concurrently into every available pilot. This enables dynamic slicing of the workload so to optimize the size, duration, and binding of pilots, and the placement of units on those pilots.

We have also used the building block approach to coordinate the distributed execution of applications with specific computational patterns. EnTK promotes ensembles as a first-class entity and has the following design features to meet the requirements of ensemble-based applications: (i) enable the expression of an ensemble of tasks abstracting the specificity of the tasks’ executables; (ii) support for the common workflow and pre-determined ensemble-based execution patterns; (iii) decoupling of the expression of patterns from the management of their execution; and (iv) a runtime system that enables the efficient execution of tasks and provides flexible resource utilization capabilities over a range of HPC platforms.

EnTK adheres to the four elements of the building block approach: It is self-sufficient as it is not limited to a specific type of ensemble or execution pattern, and thus is fully general in the scope of its entities and functionality. EnTK is interoperable across different executables and resources, supporting composability and extensibility by exposing an API tailored to the development of execution patterns, some of which are predefined for the user but which can be arbitrarily extended.

It is important to note how each RADICAL-Cybertool has been designed to be used independently. Each cyber-tool is not designed as part of an overall system: each mod-

Figure 2: Primary functional levels. The diagram supports an analysis of the functional requirements for workflow systems, and the primary entities at each level, agnostic of the applications and resources.
ule is a system in itself. Several independent communities directly utilize RADICAL-SAGA without using RADICAL-Pilot, and other communities have been using RADICAL-SAGA with alternative pilot systems implementations. This is the essence of the building block approach we are proposing. Progressively, each cybertool will be further developed to be used by a diverse research communities and with diverse workflow, pilot, manager, or broker systems.

RADICAL-Cybertools do not implement new types of system. Workflow, workload, and execution managers are common modules of many middleware supporting the distributed execution of workloads and workflows. The novelty rests with their design approach, not with their functionalities. Their adoption by a wide range of end users but also by projects that have already developed their own software modules is a testament to the relevance of the approach here proposed. We discuss details of their uptake in the next section.

4. CASE STUDIES

In this section, we discuss four case studies in which RADICAL-Cybertools have been independently integrated with user-facing libraries and production-grade systems developed by distinct teams at different institutions and from a range of disciplines. Where the same RADICAL-Cybertools module have been used across different case studies, the points of integration have been different. These case studies illustrate how the building blocks approach enables integration by implementing minimal new functionalities.

The first case study involves domain-specific workflow (DSW) systems from biomolecular sciences and seismology integrated with the EnTK module of RADICAL-Cybertools. The second and third case studies review the integration of the two workflow systems Swift [8] and FireWorks [21] with RADICAL-WLMS [14]. The fourth case study describes the integration of PanDA [22] with the Next Generation Executor (NGE) module.

The level at which systems are integrated differs in each case study. The first case study integrates four DSW systems with a single workflow manager; the second a workflow manager with an execution manager; the third an execution manager with a resource manager; and the fourth a broker with a pilot system. Further, each integration uses a different type of interface: API, file system, methods, and database. Finally, each integration implements a different element of a coordination protocol by passing tasks to a workflow manager, a master process, a resource, or a pilot.

The entities ‘task’, ‘pilot’, and ‘resource’ remain invariant across the integrations. This avoids reimplementation of functionalities in favor of translation layers among, for example, data structures representing tasks properties and relations, or resource requirements and capabilities. It should be noted that while these entities are specific to the domain of workflow and workloads, the building block approach can be used in every domain with a well-defined set of entities.

4.1 DSW Systems and EnTK

EnTK, described in the previous section, has been used to build four DSW systems to support workflows that are characterized by different ensemble- based execution patterns (Figure 3). EnTK is agnostic to the details of both the specific executables run by the ensemble and the system used to manage their execution. In Figure 3 EnTK is coupled with RADICAL-Pilot to execute the ensembles via pilots on HTC but, in principle, EnTK could use a different runtime system.

EnTK was used to build the ExTASY toolkit [23], a DSW that supports several sampling methods in biomolecular simulations. ExTASY invokes EnTK as a Python library and uses the Ensemble API to provide the simulation-analysis execution pattern. Several sampling algorithms (LSDMap and CoCo) are consistent with this execution pattern and are implemented using ExTASY.

EnTK also supports the replica-exchange pattern, and is thus usable by RepEx [24] which is a DSW enabling multiple replica-exchange methods. RepEx has been shown to be a powerful framework to support multi-dimensional and exchange schemes [25]. RepEx achieves this by separating the performance layer from the functional layer, while providing simple and easy methods to extend interfaces.

Two additional DSW use EnTK: The first is the High-throughput binding affinity calculator (HTBAC) which is used to determine clinically relevant binding affinities [26]. The other is SeisFlows [27], an open source seismic inversion package that delivers customizable waveform inversion workflows so as to support research in regional, global, and exploration seismology.

HTBAC implements the ESMACS and TIES protocols to calculate binding free energies [28]. These workflows consist of consecutive MD runs (for example equilibration and production) followed by post processing steps. Although ESMACS and TIES methods are similar at a high-level, i.e., they are comprised of concurrent, multi-stage pipelines with synchronization, they differ in the details of the pipelines, stages and synchronization. HTBAC uses the EnTK API to express these workflows; EnTK provides advanced resource management capabilities and, thereby delivers the necessary high-throughput capabilities required. EnTK provides a common API, execution and programming model to these different methods, and thus will minimize development effort and complexity.

SeisFlows is designed to support seismic inversion workflow, at scale on HPC machines. The workflow is comprised of multiple sequential and concurrent stages of the work-
flow and associated data movement which are supported using EnTK. The associated tool—SeisFlows—is used for fast prototyping of seismic workflows uses RADICAL-SAGA to extract information from a database to execute jobs. It is mostly used to run data pre-processing and simulations sub-workflows.

All four DSW systems (ExTASY, RepEx, HTBAC and SeisFlows) benefit from the use of EnTK by not having to reimplement workload management, efficient task management and interoperable task execution on distinct and heterogeneous platforms. This in turn enables both a focus on and ease of “last mile customization” for the DSW.

4.2 Swift and RADICAL-WLMS

For our study, we choose Swift, which is both a language and a runtime system to specify and execute workflows. Swift has a long development history, with several versions that supported diverse case studies. Swift also integrated pilot systems of which Coasters [29] is actively supported. The design of Swift is modular and it relies on connectors to interface with third-party systems.

In Swift, the language interpreter and the workflow engine are tightly coupled but connectors can be developed to stream the tasks of workflows to other systems for their execution. As seen in the previous section, all RADICAL-Cybertools can get streams of tasks as an input: RADICAL-SAGA can submit these tasks as jobs to diverse resources; RADICAL-Pilot can schedule these tasks into pilots; and RADICAL-WLMS can derive and enact a suitable execution strategy to execute the given tasks. Each RADICAL-Cybertools offers a different and well-isolated set of capabilities, depending on the specific set of abstractions they implement.

We integrated Swift with RADICAL-WLMS to enable the distributed and concurrent execution of Swift workflows on diverse resources (Fig. 1). The execution strategies of RADICAL-WLMS offered the possibility to minimize the time to completion of these distributed executions, obtaining both qualitative and quantitative improvements [30]. Qualitatively, RADICAL-WLMS enabled Swift to execute workflows concurrently on both HPC and HTC resources, via late binding of both tasks to pilots and pilots to resources. Quantitatively, the time to completion of workflows was improved by leveraging the shortest queue time among all the target resources.

The integration with RADICAL-WLMS required the development of a dedicated connector for Swift by iterating on the already available shell connector. The RADICAL-WLMS connector enabled saving task descriptions on the local filesystem from where RADICAL-WLMS was able to load and parse these descriptions without needing any added functionality. This type of integration was not made possible by an API—otherwise a common implementation detail— but by sharing the task entity between the two systems and by isolating distinct functionalities operating on that entity in two distinct software modules.

Both Swift and RADICAL-WLMS are examples of building blocks for L3 (as depicted in Fig. 2) but most of their components are not. For example, the workflow management component of Swift or the execution manager component of RADICAL-WLMS are not designed to be self-sufficient and extensible system that can be extended and composed with other building blocks. Swift and RADICAL-WLMS’ components can work only within those systems because they depend on private APIs and assume specific coordination and communication protocols.

4.3 FireWorks and RADICAL-Pilot

Fireworks is a workflow system with a large userbase and that enables executing workflows on distributed and sometimes large scale compute resources [21].

The design of FireWorks minimizes architectural and implementation complexity while maximizing fault-tolerance and generality of workflow descriptions. The system comprises four main components: a user-facing command-line tool to describe workflows (lpad); a database where to store one or more workflows (launchpad); a command-line tool to launch the execution of the workflows (launch); and a set of remote workers that execute the tasks of the workflows on one or more resource (rockets).

When distributing the execution of workflows’ tasks over resources, FireWorks can benefit from late binding of tasks to resources. Nonetheless, FireWorks does not implement pilot capabilities and therefore cannot late bind tasks on HPC resources. This greatly reduces the potential of using HPC resources, including the inability to support the high-throughput execution of MPI-based simulations [22].

The integration of FireWorks with RADICAL-Pilot provides these pilot capabilities. The two systems can be integrated at several levels (e.g., by sharing their database or by replacing the existing FireWorks’ workers) but by enabling FireWorks’ workers to submit jobs to RADICAL-Pilot (Fig. 5), the isolation of states and the assumptions behind FireWork’s scheduling functionalities remain unaltered.

Unlike Swift, FireWorks does not offer a adapter subsystem but a worker can be used to run a command via the RADICAL-Pilot API instead of a command to immediately execute a task. In this way, RADICAL-Pilot behaves like an independent subsystem that does not need to share any state but the initial and final with FireWorks: Failures, rescheduling, resource selection, or the multi-stage scheduling via pilots remain self-contained functionalities of RADICAL-Pilot.

This case study confirms the ‘agnosticism’ of modules designed as building blocks towards API and integration.
4.4 PanDA and NGE

PanDA is a Workload Management System designed to support the distributed execution of workflows via pilots [4]. Pilot-capable WMS enable high throughput of tasks execution via multi-level scheduling while supporting interoperability across multiple sites. PanDA WMS consists of several interconnected subsystems, communicating via dedicated API or HTTP messaging and implemented by one or more modules.

PanDA is primarily designed to support execution of independent tasks on Grid computing infrastructures like WLCG, but several prototypes have been developed to support alternative platforms. Among these, leadership-class computing systems are particularly promising as they typically run at 90% of their total yearly capacity. For example, the spare capacity of ORNL’s Titan supercomputer is equivalent to roughly 10% of the 300,000 cores used by PanDA on WLCG every year.

The use of leadership HPC machines for executing a very large amount of small jobs presents several challenges. Among those, the two most relevant are: coping with a queue system designed for large MPI jobs; and accessing the untapped resources without disrupting the overall utilization of the machine. Pilots can address the former while backfilling can be used for the latter. Pilots can be difficult to deploy on HPCs because of the token-based authentication model and the limited or absent WAN connectivity from the compute nodes. Utilizing backfilling requires in turn dedicated API or HTTP messaging and implemented by one or more modules.

PanDA Broker and NGE integrate via a database and a coordination protocol based on exchanging information exclusively about tasks and resources (Fig. 6). In this way, NGE behaves like a resource queue for PanDA Broker while the broker is a source of tasks specifications and resource requirements for NGE. Both systems require no modifications to be integrated but the development of an API to pull and poll the database.

As with Swift and FireWorks, PanDA Broker is also developed by a dedicated team, different from the one developing the RADICAL-Cybertools stack. The two teams did not coordinate their design or development effort and the integration was performed when the two stacks were already in production. Both systems implement a design compatible with the building block approach, enabling their integration. Nonetheless, their components are still tightly coupled and interdependent: for example, the Agent of RADICAL-Pilot cannot be used in isolation from the Unit and Pilot Managers and PanDA Broker cannot be used without a PanDA Server and, to some extents, outside the boundaries of the ATLAS experiment.

4.5 Analysis

These four case studies show the potential for a set of software modules to be designed without buying into the specific assumptions of a class of use cases or types of resources. These assumptions have lead to several software ecosystems that, while highly modular, do not allow reuse outside their boundaries. We believe this is why functionalities pertaining to domain-specific entities (e.g., tasks, pilots) are often reimplemented in use case-specific software systems. Each system serves well the single research group or the largest scientific project but not each other.

As argued in Section 2, software modules should be self-sufficient, interoperable, composabile, and extensible so to be able to serve a set of arbitrary requirements for a well-defined set of entities. For example, a workflow manager should provide methods for DAG traversing independent of
how and when the DAG is specified or where the tasks of the workflow will be executed. Analogously, a pilot agent module should provide multi-staging and task execution capabilities independent on the system that will schedule tasks on that agent or on the compute resources on which tasks will be executed.

Modularity is not a design principle strong enough to realize this type of software modules. Modularity needs to be augmented by API and coordination agnosticism alongside an explicit understanding of the entities that define the domain of utilization of the software system. Each module developed following this approach, implements a well-defined set of functionalities specific to a set of entities, with minimal assumptions about the system that will use these functionalities or the environment in which they will be used.

This approach is by no means a design idealization or a complete novelty. Systems like Celery, Dask, Kafka, or Docker are early examples of modules designed by implicitly following what we have here called the building block approach. These tools implement specific capabilities like queuing, scheduling, streaming, or virtualization for the domain of distributed computing. Consistently, they assume a set of core entities like concurrency, workloads, tasks, pipelines, or messages. Their composability in multiple domains and ongoing extensibility shows the potential of their underline design approach.

5. DISCUSSION

In Section 2 we described our interpretation of the building blocks approach to design distributed systems and, in particular, workflow systems. In Section 3 we illustrated how RADICAL-Cybertools were implemented in accordance to this approach. Section 4 discussed the use of RADICAL-Cybertools to constructing domain-specific workflow systems and integrating legacy systems. There, we emphasized the ability to support a wide range of scientific domains and applications with minimal perturbation and maximal reuse of functionality and software.

This paper offers four main contributions: (i) Defining the principles of self-sufficiency, interoperability, composability and extensibility that characterize a building blocks approach to the design of distributed systems; (ii) Illustrating a set of building blocks that enable multiple points of integration, which results in design flexibility and functional extensibility, as well as providing a level of “unification” in the conceptual reasoning (e.g., execution) across otherwise very different tools and systems; (iii) Showing how these building blocks have been used to develop and integrate workflow systems; (iv) the beginning of an investigation about an alternative and conceptual approach to (re)thinking the design and implementation of workflow systems and the applicability and potential of the building blocks approach.

The case studies we presented in Section 6 highlight the practical impact of the building blocks approach. The first case study, based on the integration of EnTK and RADICAL-Pilot, illustrates how well-scope building blocks can support four domain-specific workflow systems, tailored to the many distinct ensemble applications required by biomolecular sciences and seismology. The three subsequent case studies show integration to provide missing or improved functionality with widely used workflow systems and a workload management system. The integration requires minimal development, mainly focused on translation layers, and no refactoring. Together, these four case studies meet the qualitative and quantitative requirements of a variety of usage modes, a testament to the potential and impact of the building block approach.

It is important to outline what this paper does not attempt to achieve. The work captured in this work is not complete, in fact, it is a preliminary study focused on one approach to building blocks for workflows systems, without an encompassing analysis of application requirements. Although preliminary, this work is not premature: Conceptual formalisms that are too far ahead of proof-of-concepts and demonstrable advantages are unlikely to yield practical advances. Thus, even though the building blocks approach is still a work in progress, we believe early demonstrations of success are necessary. Our work also does not attempt to distinguish (or identify) either the set of applications or systems where a building blocks approach will surpass alternative approaches. Finally, our paper does not analyze the wider implications for the middleware ecosystem for scientific computing. We will address these issues and more in future work.

The building blocks approach spawns many new questions. A prominent one pertains to the issue of how we might model workflows systems and tools, so as to provide a common vocabulary, reasoning and comparative framework. The P^4 model provided this capability for the pilot abstraction [19], however it is still unclear what an analogous conceptual model of workflow systems might entail or, given the very broad diversity of workflow systems and tools, whether we can even formulate a single conceptual model. This model has been elusive so far, but might it be more fruitful to formulate a series of models of functional modules that have the properties of building blocks as defined in Section 2?

There have been many surveys and analysis of workflow management systems [31, 32, 33] which have focused on a functional analysis of workflows and classification of workflows systems. To the best of our understanding, a survey that has examined workflow systems from a software engineering perspective and practice is conspicuous by its absence. An end-goal and intended outcome of this paper is to begin a discussion on how the scientific workflows community—end-users, workflow designers when distinct from end-users, and workflow systems developers—can better coordinate, cooperate, and reduce redundant and unsustainable efforts. We believe the building blocks approach is a start toward an examination and investigation of design principles and architectural patterns for workflow systems that may facilitate this discussion.

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