Toward Common Components for Open Workflow Systems

Jay Jay Billings
Oak Ridge National Laboratory and The Bredesen Center for Interdisciplinary Research and Graduate Education,
The University of Tennessee - Knoxville
Oak Ridge, TN, USA
billingsjj@ornl.gov\Twitter:@jayjaybillings

Shantenu Jha
Computational Science Initiative, Brookhaven National Laboratory and Rutgers University
Upton, NY, USA
shantenu.jha@rutgers.edu

ABSTRACT
The role of scalable high-performance workflows and flexible workflow management systems that can support multiple simulations will continue to increase in importance. For example, with the end of Dennard scaling, there is a need to substitute a single long running simulation with multiple repeats of shorter simulations, or concurrent replicas. Further, many scientific problems involve ensembles of simulations in order to solve a higher-level problem or produce statistically meaningful results. However most supercomputing software development and performance enhancements have focused on optimizing single-simulation performance. On the other hand, there is a strong inconsistency in the definition and practice of workflows and workflow management systems. This inconsistency often centers around the difference between several different types of workflows, including modeling and simulation, grid, uncertainty quantification, and purely conceptual workflows. This work explores this phenomenon by examining the different types of workflows and workflow management systems, reviewing the perspective of a large supercomputing facility, examining the common features and problems of workflow management systems, and finally presenting a proposed solution based on the concept of common building blocks. The implications of the continuing proliferation of workflow management systems and the lack of interoperability between these systems are discussed from a practical perspective. In doing so, we have begun an investigation of the design and implementation of open workflow systems for supercomputers based upon common components.

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1 INTRODUCTION
Suppose for a moment that there is an interesting activity that would benefit from automation, which is known because the activity exhibits the following properties:

• The goal of the activity is known and desirable.
• The tasks to achieve the goal and complete the activity are also known and, furthermore, highly repetitive even in cases where decisions must be made to continue.
• The results of achieving this goal can be consumed or processed in standard ways.

This example may be recognized by many as a description—but not a definition—of a workflow. Experts from many backgrounds can easily think of activities that fit this description and even systems that automate the activity. However, each expert will probably also imagine a different workflow: a businessperson might imagine the workflow for processing payments; a medical professional might imagine updating medical charts and records; and scientists might imagine performing an analysis with modeling and simulation software, analyzing a large amount of data, or quantifying uncertainty. Within the scientific community this has led to a rather predictable situation: Everyone has a different definition of workflow and has created their own systems for managing and processing workflows.

This leads to some very practical consequences for scientific workflows. In spite of the similarities in high-level abstractions and higher-order concepts, extremely specialized software solutions and communities have developed to process scientific workflows. These differences hold across scientific problems, all generally providing some level of service that was not or perhaps is not available in a regular programming language, system library, or problem-solving workbench. These systems have accreted workflow management capabilities over time that have effectively resulted in the creation of large, monolithic software stacks that cannot communicate between each other, require a very large amount of expertise to use, often put very high demands on back-end systems either by design or through assumptions, and are often too specialized to jump between workflow execution for data analysis and modeling and simulation.

Recent developments suggest that this may be neither desirable nor necessary. The continued scalability, sophistication, and
maintainability of large, monolithic systems is called into question as scientific problems become more complex, functionality moves from libraries to operating systems, and open source development continues to rise as the dominant means of collaborating on software development. Software complexity, in particular, often makes it impossible for development on large systems to scale to the required level because the accretion of new capabilities means managing larger pools of people and a larger software development effort. One obvious alternative with some degree of historical precedence in the field is to develop common building blocks that provide common services used to both define and execute workflows. Such an approach not only makes it possible to coalesce around a standard definition and understanding of workflows, but also make it possible to separate and distribute the work required to construct the building blocks from the effort to define workflows and to create workflow management systems that may share the building blocks while retaining required customizations. This article contributes to the ongoing discussion by providing

- an illustration of the diverse nature of scientific workflows (§2) that describes the different areas where scientific workflows and systems have appeared in the literature, how they have been classified in the past, and the arguments around coalescence that are driven by calls of interoperability (§3.2 and §4);
- a description of the necessary subset of functionality that is common across a number of scientific workflow management systems that would, in principle, be good candidates for consolidation and sharing (§5); and
- an understanding of these common elements as building blocks and how composing these building blocks addresses a number of the problems not easily addressed by the monolithic design of existing systems (§5 and §6).

2 THE DIVERSITY OF WORKFLOW MODELS

One of the most challenging aspects of studying workflows is the way the vocabulary has been unintentionally overloaded. It is clearer to understand it by starting from a historical perspective. The use and study of workflows and the initial implementation of workflow management systems (i.e., systems that manage one or more activities related to workflows), and especially workflow execution, was developed in the business world to address the need to automate business processes. Ludäscher et al. ascribe the origins of workflows and workflow management systems to “office automation” trends in the 1970s [Ludäscher et al. 2006]. Van Der Aalst argues that “workflows” arose from the needs of businesses to not only execute tasks but also “to manage the flow of work through the organization,” and managing workflows is the natural evolution from the monolithic applications of the 1960s to applications that rely on external functionality in the 1990s [Van Der Aalst 1998]. By 1995, in the presence of many workflow tools, the Workflow Management Coalition had developed a “standard” definition of workflows [Hollingsworth and Hampshire 1993]:

A workflow is the automation of a business process, in whole or part, during which documents, information or tasks are passed from one participant (a resource; human or machine) to another for action, according a set of procedural rules.

In the early 2000s, workflow systems started finding use in scientific contexts where process automation was required for scientific uses instead of traditional business uses. At the time, the focus of scientific workflows also shifted to focus primarily on data processing and managing heterogeneous infrastructure for large “grids” of networked services [Yu and Buyya 2005]. Yu and Buyya define a workflow as

... a collection of tasks that are processed on distributed resources in a well-defined order to accomplish a specific goal.

This latter definition is important because of what is missing: the human element. For many in the grid/eScience workflows community this has become the standard definition of a workflow and the involvement of humans results not in a single workflow, but multiple workflows spanned by a human. Machines or instruments are absent from the definition as well, but in practice many modern grid workflows are launched automatically when data “comes off” of instruments because they remain the primary source of data in grid workflows (cf. [Megino et al. 2015]).

In addition to grid workflows, the scientific community started exploring “modeling and simulation workflows” which focus not on data flow but on the orchestration of activities related to modeling and simulation instead, sometimes on small local computers, but often on the largest of the world’s leadership class supercomputers. Unlike grid workflows they tend to require human interaction in one way or another. Some of these workflows are defined in the context of a particular way of working, such as the Automation, Data, Environment, and Sharing model of Pizzi et al. [Pizzi et al. 2016], the Design-to-Analysis model of Clay et al. [Clay 2015], or the model of Billings et al. [Billings et al. 2017].

Additional types of workflows in the scientific community include workflows that process ensembles of calculations for uncertainty quantification, verification and validation or probabilistic risk assessment [Montoya 2016], and workflows used for testing software. These workflows share the property that they are all running a very large set of coordinated jobs that only provide value when run together. However, they differ because testing workflows typically run each test as an independent task, whereas the other workflows may or may not change the tasks that are executed based on the intermediate state of the entire ensemble. These workflows require a large cluster or possibly a supercomputer in extreme cases.

Many scientific workflows have been hard-coded into dedicated environments—not general purpose workflow management systems—that serve as point solutions developed for the sole purpose of that single well-defined workflow, or at most a few, to meet the needs of a single community. This leads to an important defining characteristic for workflow management systems versus the point solutions: workflow management systems are extensible through a public application programming interface (API) or other method and extension does not, in general, require the intervention of the
original author. Embedding workflows into point-solutions may be the best solution in many cases, but the distinction between point-solutions and full workflow management systems is important because it clearly demonstrates that some parties prefer to focus on rapidly creating new or modifying old workflows, whereas others may only be interested in executing well-defined, very stable workflows.

Finally, an important class of scientific workflows is the set of “conceptual workflows” that broadly define activities based on the workflow management systems as an important part of business workflow tools employ the wrong abstraction for scientists. They There have been several efforts to classify, survey, or develop taxonomies for workflows and workflow management systems, and their inception, although not without significant overlap and duplication of effort. The survey of scientific workflow management systems by Barker and Hemert illustrates both growth and growing pains but also provides important observations and recommendations on the topic [Barker and Hemert 2007].

Barker and Hemert also provide key insights into the history of workflow management systems as an important part of business automation. The authors make an important comparison between traditional business workflow management systems and their scientific counterparts, citing in particular that traditional business workflow tools employ the wrong abstraction for scientists. They define workflows using the “standard” definition from the Workflow Management Coalition (cf. §2 above).

The discussion points that Barker and Hemert raise are important because of their continuing importance and relevance today, particularly the need to enable programmability through standard languages instead of custom proprietary languages. Sticking to standards is important and perhaps illustrated best by Barker’s and Hemert’s statement:

If software development and tool support terminates on one proprietary framework, workflows will need to be re-implemented from scratch.

This is an important point even for workflow tools that do not use proprietary standards but develop their own solutions. What can be done to support those tools and reproduce those workflows once support for continued development ends?

Montoya et al. discuss workflow needs for the Alliance for Application Performance at Extreme Scale (APEX) [NERSC 2016], and describe three main classes of workflows: simulation science, uncertainty quantification, and high throughput computing (HTC) [Montoya 2016]. HTC workflows start with the collection of data from experiments that is in turn transported to large compute facilities for processing. Many grid workflows are HTC workflows, but not all HTC workflows are grid workflows since some HTC workflows—such as those presented by Montoya et al.—may be run on large resources that are not traditionally “grid machines.” When Montoya et al. describe scientific workflows, they are referring to the modeling and simulation workflows described above. Montoya et al. also provide a detailed mapping of each workflow type to optimal hardware resources for the APEX program.

The US Department of Energy (DOE) sponsored the DOE/NGNS/CS Scientific Workflows Workshop on April 20–21, 2015. In the report, Deelman et al. describe the requirements and research directions for scientific workflows for the exascale environment [Deelman et al. 2015][Deelman et al. 2017]. The report and paper describes scientific workflows primarily by three application types: simulations, instruments, and collaborations. The findings of the workshop are comprehensive and encouraging, with recommendations for research priorities in application requirements, hardware systems, system software, workflow management system design and execution, programming and usability, provenance capture, validation, and workflow science.

The definitions of a workflow and workflow management systems are thoroughly explored and put into context for the purposes of the workshop. The authors of the report are very careful to define workflows not just as a collection of managed processes, which is common, but in such a way that it is clear that reproducibility, mobility, and some degree of generality are required by both the description of the workflow and the management system. (n.b. The report appears to provide three separate definitions for “workflow” on pages 6, 9, and 10.)

In Reference [Liew et al. 2016] Atkinson et al. discuss how to make in silico experiments more manageable by modeling them as workflows, and to use a workflow management system to organize their execution. They attribute the four primary challenges of workflow execution to (i) the complexity and diversity of applications; (ii) the diversity of analysis goals; (iii) the heterogeneity of computing platforms, and (iv) the volume and distribution of data.
They also propose a taxonomy of workflow management system characteristics.

Ferreira da Silva et al. attempt to characterize workflow management systems in [Ferreira da Silva et al. 2017]. The authors reduce key properties of workflow systems into four incongruent areas: (i) design, (ii) execution and monitoring, (iii) reusability, and (iv) collaboration. These properties are essential considerations for most software with limited specificity for workflow management systems. Furthermore, there is general conflation between classification and taxonomy and significant incoherence between entries in equivalence classes. Most significantly, it fluctuates somewhat chaotically between discussing workflows and workflow management systems without linking workflow properties to the successful design and properties of workflow systems.

3 EXPERIENCE OF A LEADERSHIP COMPUTING FACILITY

3.1 Proliferation and Common Functionality

The problems with the increase in the number of existing workflow management systems have been illustrated well by reports and discussions surrounding the future of workflow management in the leadership computing facilities. The proliferation of workflow management systems and lack of a consistent definition of a workflow are significant barriers to the adoption of this technology. There have been a number of community calls for interoperability that the problem of proliferation can be solved by consolidation of common functionality. This is typical of an operational perspective where deployment of capability is more important than in-depth investigation and research into how that capability functions.

These discussions concluded with the observation that the current proliferation of workflow systems in response to perceived domain-specific needs of scientific workflows makes it difficult to choose a site-wide operational workflow manager, particularly for leadership-class machines. However, there are opportunities where facilities can centralize workflow technology offerings to reduce anticipated fragmentation. This is especially true if a facility attempts to develop, deploy, and operate each and every workflow solution requested by the user community. Through these evaluations, the OLCF seeks to identify interesting intersections that are of the most value to OLCF stakeholders.

OLCF’s strategy is notable because it makes a very practical observation that the problem of proliferation can be solved by consolidation of common functionality. This is typical of an operational perspective where deployment of capability is more important than in-depth investigation and research into how that capability functions.

3.2 Interoperability

There have been a number of community calls for interoperability. For example, Session IV of the Twentieth Anniversary Meeting of the SOS Workshop (SOS20) focused on workflow and workflow management system development activities of the three participating institutions: Sandia National Laboratory, Oak Ridge National Laboratory, and the Swiss National Supercomputing Centre [Pack 2016]. Multiple presenters illustrated the challenges facing the workflow science community and widely agreed that no single workflow management system could satisfy all the needs of those present. Instead, attendees proposed that the community as a whole would be served best by seeking to enable interoperability where possible.

Workflow interoperability is not just a conceptual attribute, but one with important practical implications. For example, DOE Leadership Computing Facilities, as in §4, are affected by the lack of interoperability of all types. Consider the possibility that every facility may end up supporting different workflows systems entirely, so that workflows at one facility can not be run at another without significant work to install one or more additional workflow management systems! This idea is also illustrated well in The Future of Scientific Workflows report through the concept of the “large-scale science campaign” [Deelman et al. 2015]. Such a campaign integrates multiple workflows, not necessarily all in the same workflow management system or at the same facility, to perform data acquisition from experimental equipment, modeling and analysis with supercomputers, and data analysis with either grid computing or supercomputers.

4 CHALLENGES OF WORKFLOW MANAGEMENT SYSTEMS

The review of different workflow models and management systems in §2 illustrates the diversity of solutions, the lack of a coherent understanding of workflows per se, and the absence of a coordinated search for higher level concepts in spite of very good past efforts. That is, there is no standard model that describes what a workflow is, the common elements of workflow management systems, or the description of how the pieces of such a system interact to execute a workflow. Furthermore, there are few examples of interoperability among existing systems in spite of significant community pressure and calls for cross-system workflow execution. Poor or non-existent interoperability is almost certainly a consequence of the “Wild West” state of the field.

The state of the field does not mean that there is little or no common functionality between workflow management systems in different domains. Many sources in the literature, including several cited above, indicate that the contrary is in fact true: there is significant duplication and commonality in this space. The overlap in these technologies is rarely discussed on its own merits, but instead it is commonly used to create large tables comparing different systems, as in [Ferreira da Silva et al. 2017]. This creates a scenario where more effort is spent discussing how something is accomplished versus the arguably more important question of what must be accomplished.

Expanding on the concept of what must be accomplished, some primary application (workflow) needs include (i) lowering the development burden; (ii) extensibility; (iii) transporting an application workflow to another resource, platform, or workflow system; and (iv) providing a conceptual framework or basis to decide which tools are suitable or optimal for a given workflow.

Similarly, beyond having clarity on the functional and performance capabilities of a workflow system, the primary needs of users and developers of workflow systems include (i) lowering the
need to develop components, (ii) determining which components to use and reuse, (iii) minimal perturbation and refactoring when extending or generalizing the functionality or use cases supported by a workflow system, (iv) providing constant performance across different use-case scenarios and scales.

It is worth noting that workflow systems are rarely developed to extract (enhance) performance. They are more about coordinating different functionality without loss of performance. High-performance and scalability is not often a first order concern of general workflow systems; it may however, be a first order concern of specialized workflow systems or specific components (e.g., a pilot-system that is responsible for scalable and efficient task launching and management).

A healthy balance of what versus how is important, but we propose that the discussion of how particular problems are solved in workflow science has overtaken the discussion of what must be accomplished, creating two severe problems:

- A “proliferation” of tools that largely solve the same problem in the same way, but with separate, competing implementations primarily delineated along domain, as opposed to technological, boundaries.
- A general lack of interoperability and therefore inability to address larger scientific problems using hybrid combined workflows, multifacility workflow campaigns, or heterogeneous hardware without significant reimplemention.

These two problems are closely related: Tooling proliferation might not be a problem, given sufficient resources, in the absence of calls for interoperability between systems, and interoperability might not be an issue if there were not so many existing systems. However, some of the most important aspects of these problems remain separable and should be examined as such.

Workflow interoperability is neither a simple nor singular attribute. There are at least four distinct types of interoperability that merit discussion:

1. Workflow interoperability—Sharing workflows across different science problems. This was an original motivation in the initial days of eScience and reproducible computational science. Early projects such as the MyGrid (subsequently MyExperiment) and related projects, pioneered and advanced the ability to share workflows across science domains, science problems and scientists.
2. Execution delegation—Delegating the execution of a workflow to a more capable or appropriate workflow management system. Consider, for example, the formal specification of a workflow as a directed acyclic graph and associated data descriptions, such that the specification is complete and thereby in principle executable by any capable workflow management system. Although in principle and conceptually easy, this has proven to be less successful in practice for at least two primary reasons: (i) directed acyclic graphs are a common, but not universal, formal specification of some workflows, and (ii) many specific consideration and assumptions beyond those associated with a directed acyclic graph need to be factored when executing workflows. These assumptions and specific considerations in turn are often due to inadequate infrastructure abstraction and separation of concerns.
3. Workflow system interoperability—Executing the same workflow(s) by different workflow management systems. In addition to the absence of a technical or formal basis for designing workflow management systems, the sociology of software engineering and tooling contributed to the proliferation of workflow management systems. In the presence of a proliferation of tools, there was always a principled if not a practical demand for such workflow system interoperability. However, even if initially a more “principled” form of interoperability, it can be argued that workflow system interoperability is increasingly important because of the needs and requirements of reproducible science.
4. Interchangeable workflow system components—Components that can be exchanged or used concurrently across one or more systems. Until now, this is the least articulated or argued form of interoperability. However, it is the most critical and core form of interoperability that our work suggests must be addressed, if the component based approach to workflow systems is ever to supplement monolithic workflow systems.

A primary driver for seeking interoperability across workflows systems has been the need to address larger scientific problems that can only be solved with workflows that require multiple systems for complete execution. Two successful examples of limited interoperability between workflow systems are discussed in [Brooks 2015] and [Mandal et al. 2007]. Notably both projects leveraged flavors of the Ptolemy framework, namely Triquetrum and Kepler, and delegated the execution of workflows.

5 THE SOLUTION: COMMON BUILDING BLOCKS

The two problems detailed above are side effects of the relentless march of progress. The traditional approach for building workflow systems has been to build as much of the required capability as possible into the system itself, relying very little on external services or even third party code to address pressing issues in one or more domains. However, history has shown that important high-level functionality slowly moves down the software stack and into kernels, kernel services, and system libraries. Is it better at that point to use an existing system that requires significant time and resources to learn, or to develop yet another workflow management system with common tools, implementing only the gaps instead?

The answer to this question is complicated by the fact that workflows themselves have evolved. First, contemporary workflows are often the representation of methodological advances and may be more pervasive, short-lived, and wide-ranging than traditional workflows. Further, they are no longer confined to “big science” projects because sophisticated workflows are needed by many types of scientific projects, which leads to diverse design features and thus makes it unlikely that one model will be universally applicable. The ability to prototype, test and experiment with workflows at scale suggests a need for interfaces and middleware services that
enable the rapid development of resources. The challenge is to provide these capabilities along with considerations of usability and extensibility.

Jha and Turilli discuss this trend as it relates to workflows from a cyber-infrastructure perspective and to existing large-scale scientific workflow efforts [Jha and Turilli 2016]. They propose that, while historically successful, monolithic workflow systems present many problems for users, developers, and maintainers. Instead, they propose that a new “Lego-style” approach might work better where individual building blocks of capability are assembled into the final workflow management system, subsystem, or product.

More formally, a building block is a collection of functionality commonly identified across existing workflow systems that behaves like a logically and uniformly addressable service. Table 1 lists six common types of functionality that are readily observed in workflow management systems. There are certainly additional types of functionality that are common, but for pedagogical reasons we limit the list to the most obvious choices in a quick review of the literature previously cited.

Each of the types of functionality listed in Table 1 could be developed, presumably through one or more community efforts, as a building block (even the API through some programming trickery!). Other things like programming interfaces to queuing systems, programmable pilot systems for scheduling jobs, workload balancers, and ensemble execution tools, among others, could be provided as well to create a rich ecosystem of reusable and interchangeable parts.

Reusable building blocks would greatly improve both interoperability and sustainability because they would standardize, to some degree, the programming interfaces and back-ends used by workflow management systems. To the extent that projects are willing to use common building blocks, proliferation would be fully decoupled from interoperability. Leadership computing facilities would not need to support every workflow management system, just a set of common building blocks. This is similar to how they support third-party libraries for software development: they do not support every code used on these machines, but they support a set of common libraries that the codes can use.

There is an important practical question here: Does this mean abandoning existing workflow management systems or redeveloping existing workflows? No, and in fact it may be quite practical to develop building blocks based on components of the most sophisticated workflow management systems already in existence. Furthermore, because building blocks would naturally enable interoperability, it is quite conceivable that a workflow that only executes on one system now may execute on many systems in the future with little or no modification.

A second question is whether or not building blocks represent a significantly new type of modularity versus a traditional software stack or framework. Building blocks arguably sit above these entities and have distinct conceptual and functional roles. A software stack is the full set of software, including all dependencies, for a given application or software product and a framework is the set of common functionality (APIs, not libraries) around which the product is built. On the other hand, a building block may be implemented using a framework and will have some software stack, but it will also offer a complete set of functionality that can be used directly in an application. The building block may also be offered on a different system with a different implementation (i.e., using a different software stack and framework), but neither its functionality nor service interface would change.

6 DISCUSSION AND THE ROAD AHEAD

This paper is about the practice of using workflow systems in general, as opposed to the experience of a specific workflow system. It is motivated by the widely shared perception, if not strong empirical evidence and observation that there is a problem in the current practice of workflow management systems. The paper describes a variety of problems and challenges commonly found in the workflow science space. Self-evidently, no single workflow management system will be able to address the next generation of scientific challenges and practical experience dictates that a change is necessary.

There is an important separation between the challenges of expressing workflows effectively versus a workflow system that will execute the workflow. In this paper, we do not discuss the challenges inherent in expressing workflows effectively. Further, this work is not a theoretically motivated or survey paper about models of workflows or workflow systems; although plenty of such papers exist, their impact on the practice of workflow systems has been limited.

It is illustrative if not instructive to understand the ecosystem of the Apache BigData Software Stack/Cloud Model, where there are many seemingly similar components for data-intensive workflows. The proliferation of components suggests there is a strong preference of functional specialization and diversity of use, as opposed to interoperability. Equivalently, there is a strong binding of components to platforms.

In response to the problems and experience, we propose that common components in the form of building blocks are a promising and practical solution. We suggest that a building blocks approach will solve problems of system proliferation and interoperability by harnessing and developing common functionality that exists in workflow management systems into reusable services.

An important and critical test will be to devise a validation (or negation) test for the hypothesis that a building blocks approach to workflows is in fact more scalable, sustainable and better practice than monolithic workflow systems. We do not harbor illusions that it will be easy, or that it is necessarily even possible.

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Table 1: Functionality commonly identified in workflow management systems.

| Functionality                                                                 | Description                                                                 |
|------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| Data and metadata management                                                 | Management of data, metadata, and general file input and output activities whether for internal tracking or external user consumption. |
| Workflow execution engine                                                     | The primary actor that manages the execution of the activities as provided by the workflow description. |
| Resource management and acquisition                                          | Acquisition and management of resources, whether computing or instrumentation, required for the successful execution of the workflow. |
| Task management                                                               | Primary subsystem for managing individual activities, tasks or "subworkflow" using resources provided by the task management system. This system is sometimes, but neither often nor exclusively, part of the workflow execution engine. |
| Provenance engine                                                             | System for tracking execution history, sources, and destinations of ingested and generated artifacts, execution metadata including status, general logging, and provenance-based inference tools. |
| Application programming interface (API)                                       | A non-functional element of most workflow management systems that is critical to successful deployment and maintenance of the full system as well as use as a tool for creating and executing workflows. |

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