Methods Included: Standardizing Computational Reuse and Portability with the Common Workflow Language
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ABSTRACT

A widely used standard for portable multilingual/polyglot data analysis pipelines would enable considerable benefits to scholarly publication reuse, research/industry collaboration, regulatory cost control, and to the environment. Published research that used multiple computer languages for their analysis pipelines would include a complete and reusable description of that analysis that is runnable on a diverse set of computing environments. Researchers would be able to easier collaborate and reuse these pipelines, adding or exchanging components regardless of programming language used; collaborations with and within the industry would be easier; approval of new medical interventions that rely on such pipelines would be faster. Time will be saved and environmental impact would also be reduced, as these descriptions contain enough information for advanced optimization without user intervention.

In many domains the analysis components are numerous and written in multiple different computer languages by third parties. Such multilingual workflows are common or dominant in bioinformatics, image analysis, and radio astronomy.

[PROBLEM] However, lacking a standard for reusable and portable multilingual workflows, then reusing published multilingual workflows, collaborating on open problems, and optimizing their execution would be severely hampered. Moreover, only a standard for multilingual data analysis pipelines that was widely used would enable considerable benefits to research-industry collaboration, regulatory cost control, and to preserving the environment.

Prior to the start of the CWL project, there was no standard for describing multilingual analysis pipelines in a portable and reusable manner. Even today / currently, although there exist hundreds of single-vendor and other single-source systems that run workflows, none is a general, community-driven, and consensus-built standard.
CCS CONCEPTS
• Computing methodologies → Distributed computing methodologies; • General and reference → Computing standards, RFCs and guidelines; • Applied computing → Astronomy; Earth and atmospheric sciences; Enterprise interoperability; Enterprise computing infrastructures; Life and medical sciences; Bioinformatics; Transcriptomics; Computational proteomics; Population genetics; Systems biology; Computational biology; Computational proteomics; Computational genomics; Imaging; Computational transcriptomics.

KEYWORDS
workflows, computational data analysis, CWL, scientific workflows

1 INTRODUCTION
Computational Workflows are widely used in data analysis pipelines, enabling innovation and decision-making for the modern society. But their growing popularity is also a main cause for concern: unless we standardize computational reuse and portability, the use of workflows may end up hampering collaboration. How can we enjoy the common benefits of computational workflows and also eliminate such risks?

Workflow thinking [13] introduces an abstraction that helps decouple expertise in a specific domain, for example of science or of engineering, from expertise in computing. Derived from workflow thinking, a computational workflow describes a process for computing where different parts of the process (the tasks) are interdependent, e.g., a task can start processing after its predecessors have (partially) completed and where data flows between tasks.

In many domains, workflows include diverse analysis components, written in multiple (different) computer languages, by both end-users and third-parties. Such polylingual and multi-party workflows are already common or dominant in data-intensive fields like bioinformatics, image analysis, and radio astronomy; we envision they could bring important benefits to many other domains.

To thread data through analysis tools, domain experts such as bioinformaticians use specialized command-line interfaces [10, 25] and other domains use their own customized frameworks [2, 5]. Workflow engines also help with efficient management of the resources used to run scientific workloads [6, 8].

The workflow approach helps compose an entire application of these command-line analysis tools: developers build graphical or textual descriptions of how to run these command-line tools, and scientists and engineers connect their inputs and outputs so that the data flows through. An example of a complex workflow problem is metagenomic analysis, for which Figure 1 illustrates a subset (a sub-workflow).

In practice, many research and engineering groups use workflows of the kind described in Figure 1. However, as highlighted in a recently published "Technology Toolbox" article [24] published in the journal Nature, these groups typically lack the ability to share and collaborate across institutions and infrastructures without costly manual translation of their workflows.

Currently, many competing workflow management systems and runners exist, each with their own syntax or method for describing workflows and infrastructure requirements. This limits computational reuse and portability. In particular, although the data-flows are becoming increasingly more complex, most workflow abstractions do not enable explicit specifications of data-flows, increasing significantly the costs to reuse and port the workflow by third-parties.

We thus identify an important problem for the broad adoption of workflow thinking in practice: although communities want polylingual and multi-party workflows, adopting and managing different workflow systems is costly and difficult. In this work, we propose to tame this complexity through a common abstraction that covers the majority of features used in practice, and is (or can be) implemented in many workflow systems.

In the computational workflow depicted in Figure 1, practitioners solved the problem by adopting the Common Workflow Language (CWL), an open standard for describing command-line tool based workflows like theirs. We posit in this work that CWL can help solve the main problems of sharing workflows between institutions and users. We also set out to introduce the CWL standards, with a tri-fold focus: (1) CWL focuses on maintaining a separation of concerns between the description and execution of tools and workflows; (2) CWL supports workflow automation, scalability, abstraction, provenance, portability, and reusability; and (3) CWL takes a principled, community-first open-source and open-standard approach which enables this result.

CWL is the product of an open and free standards-making community. The many CWL contributors shaped the standard so that it could be useful to any domain that experiences the problem of “many tools written in many programming languages by many parties”. CWL began in the bioinformatics domain. Since the ratification of the first version in 2016, the CWL standards have been used in other fields including hydrology1, radio astronomy2, geospatial analysis [11, 21, 26], high energy physics [4], in addition to fast-growing bioinformatics fields like genomics and cancer research [18]. The flexibility of CWL enabled [14] rapid collaboration on and prototyping of a COVID-19 public database and analysis resource.

CWL could also be useful in computational domains beyond science. The separation of concerns proposed by CWL enables diverse projects, and would also benefit engineering and large industrial projects. Likewise, users of software container technology like Docker that distribute analysis tools can use CWL for providing a structured workflow-independent description of how to run their tools, what data is required, and what results to expect.

Key Insights [in C ACM box]
Toward computational reuse and portability of polylingual, multi-party workflows, CWL makes the following contributions:

1 CWL is a set of standards for describing and sharing computational workflows.
2 CWL is used daily in many science and engineering domains, including by multi-stakeholder teams.
3 CWL has a declarative syntax, facilitating polylingual workflow tasks. By being explicit about the runtime environment

and any use of software containers, CWL enables portability and reuse. (See Section 3.)

4 The CWL standards provide a separation of concerns between workflow authors and workflow platforms. (More in Section 4.3.)

5 The CWL standards support critical workflow concepts like automation, scalability, abstraction, provenance, portability, and reusability. (Details in Section 2).

6 CWL is developed around core principles of community and shared decision making, re-use, and zero cost for participants. (Section 4 details the open standards.)

7 CWL is provided as freely available open standards, supported by a diverse community in collaboration with industry, and is a Free/Open Source Software ecosystem (see Sidebar B, Section 4.2).

2 BACKGROUND ON WORKFLOWS AND STANDARDS FOR WORKFLOWS

Workflows, and standards-based descriptions thereof, hold the potential to solve key problems in many domains of science and engineering. This section explains why.

2.1 Why Workflows?

Using workflow techniques, especially with digital analysis processes, has become quite popular and does not look to be slowing down: one platform recently celebrated its 10,000th citation\(^1\); and over 294 computational workflow systems are known\(^2\). Why are workflows needed?

Workflows address two key problems. First, a process, digital or otherwise, may grow to such complexity that the authors and users of that process have difficulties in understanding its structure, scaling the process, managing the running of the process, and keeping track of what happened in previous enactments of the process. Process dependencies may be undocumented, obfuscated, or otherwise effectively invisible; even an extensively documented process may be difficult to understand by outsiders or newcomers if a common framework or vocabulary is lacking. The need to run the process more frequently or with larger inputs is unlikely to be achieved by the initial entity (i.e., either script or person) running the process. What seemed once a reasonable manual step (run this command here and then paste the result there; then call this person for permission) will, under the pressure of porting and reusing, become a bottleneck. Informal logs (if any) will quickly become unsuitable for answering an organization’s need to understand what happened, when, by whom, and to which data.

A second significant problem is that incomplete method-descriptions are common when computational analysis is reported in academic research [15]. Reproduction, re-use, and replication [9] of these digital methods requires a complete description of what computer applications were used, how exactly they were used, and how they were connected to each other. For precision and interoperability, this description should also be in an appropriate standardized machine-readable format.

Workflow techniques aim to solve these problems by providing the Abstraction, Scaling, Automation, and Provenance (A.S.A.P.) features [7]. Workflow constructs enable a clear abstraction about the components, the relationships between components, and the inputs and outputs of the components turning them into well-labeled

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1https://galaxypoint.org/blog/2020-06-10k-pubs/
2https://s.apache.org/existing-workflow-systems
tools with documented expectations. This abstraction enables scaling (execution can be parallelized and distributed), automation (the abstraction can be used by a workflow engine to track, plan, and manage execution of tasks), and provenance tracking (descriptions of tasks, executors, inputs, outputs; with timestamps, identifiers, and other logs, can be stored in relation to each other to later answer structured queries).

Sharing workflow descriptions based on standards addresses the second problem: the availability of the workflow description provides needed information when sharing; and the quality of the description provided by a structured, standards-based approach is much higher than the current approach of verbal descriptions in scientific reports. Moreover, the operational parts of the description can be provided automated by the workflow management system, rather than by domain experts.

2.2 Why Workflow Standards?

Although workflows are very popular, currently every workflow system is incompatible with the others—except for systems adopting the CWL standards. This means users are required to express their computational workflows in a different way every time they have to use another workflow system. Local success, global unportability. Could the (CWL) standards provide a better way?

The success of workflows is now their biggest drawback: users are locked into a particular vendor, project, and often a particular hardware setup. This hampers sharing and re-use. Even non-academics suffer of this situation, as the lack of standards (or the lack of their adoption) hinders effective collaboration on computational methods within and between companies. Likewise, this unportability affects public-private partnerships and the potential for technology transfer from public researchers.

A standard for sharing and reusing workflows can provide a solution to describing portable, re-usable workflows while also being workflow-engine and vendor-neutral.

2.3 Sidebar A: Monolingual and Polylingual workflow systems

Workflows techniques can be implemented in many ways, i.e., with varying degrees of formalism, which tends to correlate with execution flexibility and features. Typically, whereas the most informal techniques require that all processing components are written in the same programming language or are at least callable from the same programming language, the formal workflow techniques tend to allow components to be developed in multiple programming languages.

Among the informal techniques, the do-it-yourself approach uses from a particular programming language its built-in capabilities. For example, Python provides a threading library, and the Java-based Apache Hadoop [27] provides MapReduce capabilities. To gain more flexibility when working with a particular programming language, general third-party libraries, such as ipyparallel6, can enable remote or distributed execution without having to re-write one’s code.

A more explicit workflow structure can be achieved by using a workflow library focusing on a specific programming language.

For example, in Parsl [2], the workflow constructs ("this is a unit of processing", "here are the dependencies between the units") are made explicit and added by the developer to a Python script, to upgrade it to a scalable workflow. (We list here Parsl as an example of a monolingual workflow system, although it also contains explicit support for executing external command-line tools.)

Two approaches can accommodate polylingual workflows where the components are written in more than one programming language, or where the components come from third-parties and the user does not want to or cannot modify them: use of per-language add-in libraries or the use of the Portable Operating System Interface command-line interface (POSIX CLI) [12]. The use of per-language add-in libraries entails either explicit function calls (e.g., using ctypes in Python to call a C library6) or the addition of annotations to the user’s functions, and requires mapping/restricting to a common cross-language data model.

Essentially all programming languages support the creation of POSIX CLIs familiar to many Linux and macOS users; scripts or binaries which can be invoked on the shell with a set of arguments, reading and writing files, and executed in a separate process. Choosing the POSIX command-line interface as the point of coordination means the connection between components is done by an array of string arguments representing program options (including paths to data files) along with a string-based environment variables (key-value pairs). This command-line option has the advantage of not needing per-language implementation at the expense of a very simple data model (and process start-up costs) which in workflows leads to a tendency for larger granularity of the units of work. (As a polylingual workflow standard, CWL uses the POSIX CLI data model.)

3 FEATURES OF THE COMMON WORKFLOW LANGUAGE STANDARDS

CWL supports polylingual and multi-party workflows, for which it enables computational reuse and portability (see also the CACM Box for main features). To do so, each release of CWL has two main components: (1) a standard for describing command line tools; and (2) a standard for describing workflows that compose such tool descriptions. The goal of the CWL Command Line Tool Description Standard is to describe how a particular command line tool works: what are the inputs and parameters and their types; how to add the correct flags and switches to the command line invocation; and where to find the output files. As shown in Figure 2B, item 3, these tool descriptions can contain hints such as which software container to use or how much compute resources are required (memory, number of CPU cores, disk space, and/or the maximum time or deadline to complete the step or entire workflow.)

CWL is an explicit language, both in syntax, and in its data and execution model. The textual syntax is derived from YAML7. The syntax does not restrict the amount of detail; for example, Figure 2A depicts a simple example with sparse detail, and Figure 2B depicts

6https://docs.python.org/3/library/ctypes.html
7A third component also exists, Schema Salad, the corresponding schema language standard that is used to define the syntax of CWL itself.
8https://www.commonwl.org/v1.2/CommandLineTool.html
9JSON is an acceptable subset of YAML, and common when converting from another format to CWL.

Methods Included: Standardizing Computational Reuse and Portability with the Common Workflow Language

the same example but with the execution augmented with further details. Each input to a tool has a name and a type (e.g., File, see label 1 in the figure). Authors of tool descriptions are encouraged to include documentation and labels for all components (i.e., as in Figure 2B), to enable the automatic generation of helpful visual depictions and even Graphical User Interfaces for any given CWL description. Metadata about the tool description authors themselves encourages attribution of their efforts.

The CWL execution model is explicit: Each tool’s runtime environment is explicit and any needed elements must be specified by the author of the CWL tool-description\(^\text{10}\). Each tool invocation uses a separate working directory, populated according to the CWL tool description, e.g., with the input files explicitly specified by the workflow author. For executing more “opinionated” applications, additional CWL constructs allow further customization of the runtime environment, e.g., particular file layout, additional static files, and environment variables.

The explicit runtime model enables portability, by being explicit about data locations. As Figure 3 indicates, this enables execution of CWL workflows on diverse environments as provided by various implementations of the CWL standards: the local environment of the author-scientist (e.g., a single desktop computer, laptop, or workstation), a remote batch production-environment (e.g., a cluster, an entire datacenter, or even a global multi-datacenter infrastructure), and an on-demand cloud environment.

CWL supports explicitly the use of software container technologies, such as Docker and Singularity, to enable portability of the underlying analysis tools. Figure 2B, item 2, illustrates the process of pulling a Docker container-image from the Quay.io registry; then, the workflow engine automates the mounting of files and folders within the container. The container included in the figure has been developed by a trusted author and is commonly used in the bioinformatics field with an expectation its results are reproducible. Indeed, the use of containers can be seen as a confirmation that a tool’s execution is reproducible, when using only its explicitly declared runtime-environment. Similarly, when distributed execution is desired, no changes to the CWL tool-description are needed: because the file or directory inputs are already explicitly defined in the CWL description, the (distributed) workflow platform can handle (without additional configuration) both job placement and data routing between compute nodes.

The Common Workflow Language standards aim to cover the common needs of users and the commonly implemented features of workflow runners or platforms. To support features that are not in the CWL standards, CWL provides well-defined extension

\(^\text{10}\)https://www.commonwl.org/v1.2/CommandLineTool.html#Runtime_environment

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Figure 2: Example of CWL syntax and progressive enhancement. (A) and (B) describe the same tool, but (B) is enhanced with additional features: human-readable documentation, file format identifiers validation of workflow connections; recommended software container image for more reproducible results and easier software installation; dynamically specified resource requirements to optimize task scheduling and resource usage without manual intervention. The resource requirements are expressed as hints.
points that permit (namespaced) vendor-specific features in explicitly defined ways. If these extensions do not fundamentally change how the tool should operate, then they are marked as hints and other CWL engines can ignore them. However, if the extension is required to properly run the tool being described, e.g., due to the need for some specialized hardware, then the extension is listed under requirements and CWL engines can recognize and explicitly declare their inability to execute that CWL description.

The CWL Workflow Description Standard\(^{11}\) builds upon the CWL Command Line Tool Standard: it has the same YAML- or JSON-style syntax, with explicit workflow level inputs, outputs, and documentation (see Figure 2). The workflow descriptions consists of a list of steps, comprised of CWL CommandLineTools or CWL sub-workflows, each re-exposing their tool's required inputs. Inputs are connected from either the common workflow inputs or from outputs of other steps. The workflow outputs expose selected outputs from workflow steps, making explicit which intermediate step outputs will be returned from the workflow. All connections include identifiers, which CWL document authors are encouraged to name meaningfully, e.g., `reference_genome` instead of `input7`.

CWL workflows form explicit data flows, as required for the particular computational analysis. The connectivity between steps defines the partial execution order. Parallel execution of steps is permitted and encouraged whenever multiple steps have all of their inputs satisfied, e.g., in Figure 1, `find_16S_matches` and `find_S5_matches` are at the same data dependency level and can execute concurrently or sequentially in any order. Additionally a scatter construct allows the repeated execution of a CWL step to iterate or select from input arrays, or from multiples links to the same input. Starting with CWL version 1.2, workflows can also conditionally skip execution of a (tool or workflow) step, based upon a specified intermediate input or custom boolean evaluation. Combining these features allows for a flexible branch mechanism that allows workflow engines to calculate data dependencies before the workflow starts, and thus retains the predictability of the data flow paradigm.

In contrast to hard-coded approaches that rely on implicit file-paths particular for each workflow, CWL workflows are more flexible, reusable, and portable (which enables scalability). The use in CWL of explicit runtime environments, combined with explicit inputs/outputs to form the data flow, enables step reordering and explicit handling of iterations. The same features enable scalable remote execution and, more generally, flexible use of runtime environments. Moreover, in CWL, individual tool definitions from multiple workflows can be reused in any new workflow.

CWL workflow descriptions are also future-proof. Forward compatibility of CWL documents is guaranteed, as each CWL document declares which version of the standards it was written for and minor versions do not alter the required features of the major version. A stand-alone upgrader\(^{12}\) can automatically upgrade CWL documents from one version to the next, and many CWL-aware platforms will internally update user-submitted documents at runtime.

4 OPEN-SOURCE, OPEN STANDARDS, OPEN COMMUNITY

Given the numerous and diverse set of potential users, implementers, and other stakeholders, we posit that a project like CWL requires combined development of code, standards, and community. Indeed, these requirements were part of the foundational design principles for CWL (Section 4.1); in the long run, these have fostered free and open source software (Sidebar B, in Section 4.2), and a vibrant and active ecosystem (Section 4.3).

4.1 The CWL Principles

CWL is based on a set of five principles:

**Principle 1:** The core of the project is the community of people who care about its goals.

\(^{11}\)https://www.commonwl.org/v1.2/Workflow.html

\(^{12}\)https://pypi.org/project/cwl-upgrader/
Principle 2: To achieve the best possible results, there should be few, if any, barriers to participation. Specifically, to attract people with diverse experiences and perspectives, there must be no cost to participate.

Principle 3: To enable the most good, project outputs should be used as people see fit. Thus, the standards themselves must be licensed for reuse, with no acquisition price.

Principle 4: The project must not favor any one company or group over another, but neither should it try to be all things to all people. The community decides.

Principle 5: The concepts and ideas must be tested frequently: tested and functional code is the beginning of evaluating a proposal, not the end.

In time, the CWL project-members learned that this approach is a superset of the OpenStand Principles, a joint “Modern Paradigm for Standards” promoted by the IAB, IEEE, IETF, Internet Society, and W3C. The CWL additions to the OpenStand Principles are: (1) to keep participation free of cost, and (2) the explicit choice of the Apache 2.0 license for all its text, conformance tests, and reference implementation.

Necessary and sufficient: All these principles have proven to be essential for the CWL project. For example, the free cost and open source license (Principles 2 and 3) has enabled many implementations of the CWL standards, several of which re-use different parts of the CWL reference runner. Being community-first (Principle 1) has led to several projects that are outside the CWL standards themselves; the most important contributions have made their way back into the project (Principle 4).

As part of Principle 5, contributors to the CWL project have developed a suite of conformance tests for each version of the CWL standards. These publicly available tests were critical to CWL’s success: they helped prove the reference implementation of CWL itself; they provided concrete examples to early adopters; and they enabled the developers and users of production implementations of the CWL standards to confirm their correctness.

4.2 Sidebar B: The CWL and Free/Open Source Software (F/OSS)

4.2.1 Free and Open Source implementations of CWL

By 2021, CWL has gained much traction and is currently widely supported in practice. In addition to the implementations in Table 1, Galaxy [1] and Pegasus [8] have in-development support for CWL as well.

Wide adoption benefits from our principles: CWL offers conformance tests, but the CWL community does not yet test or certify CWL implementations, or specific technology stacks. Instead, platform/service providers self-certify support for CWL, based on a particular technology configuration they deploy and maintain.

4.2.2 F/OSS tools and libraries for working with CWL

Table 1: Selected F/OSS workflow runners and platforms that implement the CWL standards.

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Platform support</th>
</tr>
</thead>
<tbody>
<tr>
<td>cwltool</td>
<td>Linux, macOS, Windows (via WSL 2) local execution only</td>
</tr>
<tr>
<td>Arvados</td>
<td>in the cloud on AWS, Azure and GCP, on premise &amp; hybrid clusters using Slurm</td>
</tr>
<tr>
<td>Toil</td>
<td>AWS, Azure, GCP, Grid Engine, HTCondor, LSF, Mesos, OpenStack, Slurm, PBS/Torque also local execution on Linux, macOS, MS Windows (via WSL 2)</td>
</tr>
<tr>
<td>CWL-Airflow</td>
<td>Local execution on Linux, OS X or via dedicated Airflow enabled cluster.</td>
</tr>
<tr>
<td>REANA</td>
<td>Kubernetes, CERN OpenStack, OpenStack Magnum</td>
</tr>
</tbody>
</table>

CWL plugins for text/code editors exist for Atom, vim, emacs, Visual Studio Code, IntelliJ, gedit, and any text editor that support the “language server” standard.

There are tools to generate CWL from Python (via argparse/click), Python (via functions), ACD, CTD, annotations in IPython Jupyter Notebooks. Libraries to generate and/or read CWL exist in many languages: Python, Java, R, Go, Scala, and C++.

4.3 The CWL Ecosystem

Beyond the ratified initial and updated CWL standards released over the last six years, the CWL community has developed many tools, software libraries, connected specifications, and has shared CWL descriptions for popular tools. For example, there are software development kits for both Python and Java that are generated automatically from the CWL schema; this allows programmers to load, modify, and save CWL documents using an object oriented model that has direct correspondence to the CWL standards themselves. CWL SDKs for other languages are possible by extending the code generation routines.(See Sidebar B in Section 4.2.2 for practical details.)

Some workflow users require the maintenance and risk-mitigation guarantees offered by commercial operations. There are multiple commercially supported systems that support CWL for executing workflows and they are available from vendors such as Curri (Arvados), DNAnexus, IBM (IBM® Spectrum LSF), Illumina (Illumina Connected Analytics), and Seven Bridges.

CWL supports well the acute need to reuse (and, correspondingly, to share) information on workflow execution, and on authoring and provenance. The CWLProv prototype was created to show how existing standards [3, 20, 22] can be combined to represent

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13https://open-stand.org/about-us/principles/
14Snapshot of https://www.commonwl.org/Implementations
15https://github.com/common-workflow-language/galaxy/pull/47
16https://github.com/common-workflow-language/galaxy/pull/47
17Summarized from https://www.commonwl.org/#Software_for_working_with_CWL
the provenance of a specific execution of a CWL workflow[19]. Although, to-date, CWLProv has only been implemented in the CWL reference runner, interest is high in additional implementation and further development—similarly to what other CWL developments experienced during their first years of existence.

One criteria for evaluating a workflow language is the extent to which it supports a separation of concerns between the workflow description authors and the software implementers of the language. This separation of concerns is realized in CWL by using an explicit description approach. This has enabled several optimizations in scheduling (location-based [16], cost-based[17]) and data-organization by researchers and other implementers of the CWL standards.

5 CONCLUSION

The problem of standardizing computational reuse is only increasing in prominence and impact. Addressing this problem, various domains in science, engineering, and commerce have already started to migrate to workflows, but efforts focusing on the portability and even definition of workflows remain scattered. In this work we raise awareness to this problem and propose a community-driven solution.

The Common Workflow Language (CWL) is a family of standards for the description of command line tools and of workflows made from these tools. It includes many features developed in collaboration with the community: support for software containers, resource requirements, workflow-level conditional branching, etc. Built on a foundation of five guiding principles, the CWL project delivers open standards, open-source code, and an open community.

For the past six years, the community around CWL has developed organically, with plugins and converters for many systems, along with several production-grade implementations of the standards themselves.

To conclude: this is a call for others to embrace workflow thinking and join the CWL community!

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