Software publications with rich metadata

State of the art, automated workflows and HERMES concept

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Abstract

To satisfy the principles of FAIR software, software sustainability and software citation, research software must be formally published. Publication repositories make this possible and provide published software versions with unique and persistent identifiers. However, software publication is still a tedious, mostly manual process.

To streamline software publication, HERMES, a project funded by the Helmholtz Metadata Collaboration, develops automated workflows to publish research software with rich metadata.

The tooling developed by the project utilizes continuous integration solutions to retrieve, collate, and process existing metadata in source repositories, and publish them on publication repositories, including checks against existing metadata requirements. To accompany the tooling and enable researchers to easily reuse it, the project also provides comprehensive documentation and templates for widely used CI solutions. In this paper, we outline the concept for these workflows, and describe how our solution advance the state of the art in research software publication.

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Requesting community feedback

Community feedback At this stage, we would like to reach out to the community to gain insights into what desirable solutions can look like, what potential pitfalls are, etc.

We kindly ask readers and other interested parties to provide feedback on the concept detailed here via its PubPeer page at https://software-metadata.pub/concept-paper-community-reviews.

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- What metadata types, formats and standards are missing from our lists in Metadata?
- Does table 1, mapping metadata types to metadata formats, miss anything important, or misrepresent something?
- Does table 2 miss any other publication workflows you know and should be included?
- What are desired additional outputs of the automated workflows in addition to deposition in the targeted publication repositories? E.g., would the creation of CodeMeta files or Citation File Format be helpful, are there other desired output types?
- Should the HERMES pipelines leverage workflow domain specific languages (such as Common Workflow Language (CWL), Nextflow, etc.) to knit together existing tools, such as harvesters (e.g., Software Metadata Extraction Framework (SoMEF)), converters (e.g., Citation File Format Converter), and deposition tools (e.g., Zenodraft)?
- While we initially restrict the scope of HERMES with regard to metadata validation to linting (see 3.4), there may be other factors that influence the validity of metadata. It is known that VCS contributors metadata, for example, is unsuitable to be used as valid authorship metadata, as there may be people qualifying as authors who have not contributed to a source code repository, or people that are contributors but do not qualify as authors under a given definition of authorship. Therefore, other metadata sources, such as files in the Citation File Format may be more trustworthy. What are other pitfalls concerning the validity of metadata that HERMES should be aware of?

1 Introduction

There is increasing awareness that software is a valid research output and should be treated as such [21, 35]. Thus, software is increasingly published in public repositories or software journals [34]. This is a necessary step in transferring the FAIR principles to software [5] – i.e., for finding, understanding, reusing, sharing and citing software – and promoting it to first class research citizenship. Recent policy updates from universities, research institutes (e.g., at Helmholtz Association (HGF) [13]) and funders such as the Deutsche Forschungsgemeinschaft (DFG) [12] reflect this progress. Metrics for published software may inform funding decisions in the future.

The main driver for a fulfillment of the functions of FAIR software is software metadata [23], and thus, publication of research software with rich metadata is essential. In modern research software development, metadata on different software properties is created automatically, semi-automatically or manually at different stages, and in different places and formats. While this metadata can already be collected, verified and validated, and edited to be published with software, there is currently no streamlined, automated process or workflow to do so. This in turn disincentivizes the researchers, research software engineers and maintainers who create and maintain research software, to publish it with rich metadata.

In this paper, we describe a concept for automated publication of research software with rich metadata via existing automation tools. The concept is being developed in the project HERMES (HElmholtz Rich MEtadata Software Publication), conducted at the German Aerospace Center (DLR), Forschungszentrum Jülich (FZJ) and Helmholtz Zentrum Dresden Rossendorf (HZDR), and funded by the Helmholtz Association of German Research Centers' Helmholtz Metadata Collaboration (HMC) initiative (see Acknowledgments).

The work packages related to the concept as described in this document yield a number of outputs:

- **software** to retrieve existing software metadata in source code repositories, collate and process them to produce a coherent set of metadata for the current state of a given repository;
- templates, e.g. for CI/CD systems and workflow engines, to run the metadata tools on a users' source repositories;
- documentation and examples for the outputs the project provides.

In the following sections, we describe the state of the art for software metadata, available tooling to work with metadata and existing approaches to automation. We then lay out our concept for research software deposits with rich metadata in automated workflows for two target platforms. In the process, we specify requirements for the structure and contents of source code repositories, define an iterative process for the inclusion of increasingly unstructured metadata, detail the scope of the project and provide a high-level outline of the implementation of both interfaces and tooling.

We request community feedback for the concept detailed here (see community feedback above). Based on feedback we receive, the HERMES project partners design interfaces and develop software tools to automatically aggregate metadata included in software repositories. The interfaces and software tools combination provide an extensible, CI/CD-driven serverless solution that enables direct ingestion into publication repositories, such as Zenodo or Harvard Dataverse, and other repositories using the underlying InvenioRDM or Dataverse project software.

2 State of the art

2.1 Metadata

Software metadata provides information about software, or specific properties of software. It is created intentionally, or generated as a side-product during software development processes. As such, metadata can also pertain to different parts of software, or a software package as a whole. Additionally, it can exist in different modes, i.e., as structured or unstructured metadata. It may also pertain to different aspects of the software, e.g., the license regulating its use and development, its creation context, etc. Consequently, there exist different types of metadata.

Software metadata may be provided in dedicated files, or as part of some file. Metadata can also be part of version control systems or other forms of repositories, as well as the file system or platform hosting the source code. We define these as statically available metadata.

Structured metadata, especially when persisted in files, may furthermore come in specific formats. These may be standard formats through formal processes or community practice.

In this section, we describe different types of software metadata, as well as formats they are provided in. Table 1 on page 15 shows a mapping of metadata types to the formats they are commonly provided in, based on our experience.

2.1.1 Types

There are generic types of metadata that exist for software but may also be found for other digital data, as well as software-specific metadata. The latter is partly due to the fact, as described in [24], that software is both static (as source code, i.e., digital data) and dynamic (at runtime).

Generic software metadata includes:

- Software name
- File system metadata
- (e.g., file sizes, number of files, etc.)
- Authorship and contributorship information
- Reference to the documentation pertaining to the software
- Legal and licensing information
- Funding information
- Domain context
- Citation metrics
- Location metadata (e.g., download or instance URLs, etc.)
- Publication dates, etc.
- Categorization information (e.g., application category, keywords, etc.)
- Availability information (e.g., purchasing costs, etc.)
- Identifiers
- Relational metadata (e.g., software *is part of* another work)
- High-level description

Software-specific metadata includes:

- Dependency information
- Lines of code
- Programming language
- Version information (e.g., metadata from version control systems, publication platforms, or even file names; version identifiers, etc.)
- Runtime requirements, including hardware requirements
- References to work the software is built on, or relates to
- Software metrics (e.g., quality metrics like code coverage, ...)
- Development metrics (e.g., pertaining to issues, pull requests, ...)
- Usage metrics (e.g., downloads, stars, citations, ...)
- Infrastructural metadata (e.g., build and CI systems used to produce version artifacts, etc.)

2.1.2 Formats

Some metadata are persisted in files that have specific formats, or are integrated in specific formats as part of other files. Such files are usually persisted and version controlled alongside source code. Other metadata must be retrieved from third-party systems, e.g., the version control system, source code platform (GitHub, GitLab, or other), etc., if available. Some are only available on other platforms or systems and may not be retrievable from the source code repository.

Plain text files Some software metadata is provided in plain text. There are some typical dedicated plain text files, such as license files (LICENSE, REUSE Specification compliant files, etc.) or citation metadata files (plain text CITATION files), that can reasonably be assumed to contain only relevant metadata.

Other files mix metadata and other information, such as documentation files (README files and other plain text documentation), community files containing contributor information, a code of conduct, governance information, or other information. Other relevant metadata may be provided in plain text in a less overt manner, e.g., embedded in source code files.

Generally, while plain text metadata is easily accessible for human readers, they are perhaps the hardest to process using automated approaches. This is due to their less structured form and a lack of clarity with regard to semantics. A plain CITATION file, for example, may provide retrievable publication metadata, but there is no way of automatically verifying that the metadata unambiguously pertains to a specific version of the software it is provided with, or indeed something else entirely.

The same is true for any plain text metadata and specifically for metadata that are embedded in plain text: while methods exist to extract metadata from plain text, they rely on heuristics that can only produce assumptions with some degree of confidence in their significance and correct categorization.

schema.org files schema.org [17] provides schemas for structured data markup. These are commonly used in HTML to provide metadata that is reused by search engines. schema.org schemas are also used as basis for metadata in RO-Crate [37]. Additionally, there is ongoing work¹ to add missing terms from the CodeMeta schema [22] to schema.org.

CodeMeta files CodeMeta [22] is a format for generic software metadata, implemented in JSON-LD, extending schema.org files. It is used to provide comprehensive information about software, with some focus on academic use cases.

Citation File Format The Citation File Format [9] is a format to provide citation metadata for software, implemented in YAML. Its focus is exclusively to provide citation-relevant metadata in a form that is both human- and machine-readable.

Zenodo JSON files The open access publication platform Zenodo [10] uses its own metadata schema, implemented in JSON². The schema is used in practice to provide metadata for works that are being published on Zenodo, e.g., through the GitHub-Zenodo integration (see also Pull-based workflows and table 2 on page 16).

BIBTEX files BIBTEX files contain citation metadata for one or more works. The format is standardly used as input for citations and bibliographies in LATEX documents, but is sometimes also adapted to provide convenient citation metadata for software, for example in a dedicated file in source code repositories (sometimes called CITATION), or embedded in a text or marked up document such as a README file.

In the context of metadata retrieval, BIBT_EX files or snippets pose the same challenges as plain text due to their generic nature. It is hard to understand if a BIBT_EX item is describing the software package it is provided with, one of its versions, or something else entirely. The biblatex-software [7] package for IAT_EX solves issues around citing different software reference types in scholarly publications, but the general issue with BIBT_EX items and their relation to given software remains.

¹https://github.com/codemeta/codemeta/issues/232

²https://developers.zenodo.org/#github

Manifest files Manifest files describe a software package or a subunit of a software package. They exist for different programming languages and frameworks and come in a variety of implementation formats. Some examples include Project Object Model (POM) XML files for Java projects using the Apache Maven build management tool, JAR manifests for packaged Java applications, or setup.py/pyproject.toml files that contain metadata for Python packages built with Python's distutils.

Configuration files Configuration files are often added to source code repositories to leverage third-party tools such as CI/CD services or source code or documentation generators. They come in different formats, of which common ones are plaintext key-value definitions, INI, TOML, YAML, JSON and XML. Configuration files may include metadata pertaining to, e.g., software dependencies, development and publication processes, etc. One popular example for configuration files that contain contribution metadata are those for the All Contributors³ specification.

Linked Data files Linked data provides an extensible way to describe research software in depth. Common linked data formats are based on RDF [33], using serializations like JSON-LD [46] or Turtle [47]. They express not just attributes or simple relations, but reuse formalized concepts (ontologies) to describe usage, ideas, context, etc., in much greater depth than other formats listed above.

Although ontologies are a powerful concept, there does not seem to be sufficient uptake of using software ontologies to describe software in practice. This may change in the future.

Commonly known ontologies for software include Software Description Ontology [14], Software Ontology [26], SEON [49] and DOAP [48].

Version control system The version control system in use may provide valuable metadata from the commit history. Especially in distributed version control systems like Git, the complete history is available locally. These metadata are part of a project context and not formalized in a file, but may be retrieved by using command line interfaces or wrapping libraries of the version control system at hand. They may provide insights for example into contributors, file metadata, changes over time or related software/data.

Platform API responses While not strictly a format, software metadata is also available from different (e.g., REST, GraphQL) APIs, such as those for querying software development platforms (like GitHub or GitLab), WikiData, or publication repositories. These may provide metadata on software development processes, version control, contributions, publications, as well as other metadata. These APIs can usually be queried through their endpoints – or globally using a common query language such as [44] – and responses are usually provided as JSON or XML that can easily be persisted and reused.

2.2 Standards

As of now, there are no software metadata formats relating to our work that are formally standardized and cover HERMES' scope completely. Some de facto standards exist:

- CodeMeta's ongoing integration⁴ into schema.org promises at least future de facto standardization.
- The DataCite Metadata Schema [16], although used widely, has a much more generic scope again than, e.g., CodeMeta, and does not implement as large a vocabulary pertaining to software (see the CodeMeta-DataCite crosswalk⁵).

Standards in similar stages exist in related areas, such as for research objects in general:

- RO-Crate [37] packages research objects with their metadata, its schema based on schema.org.
- BagIt [25] is a generic packaging standard used in, e.g., libraries, to package file structures with metadata, where the metadata schema is very generic and not targeted to software specifically.

³https://allcontributors.org

⁴https://github.com/codemeta/codemeta/issues/232

⁵https://codemeta.github.io/crosswalk/datacite/

2.3 Integrations

Some platforms and tools provide integrations for some of the above-mentioned formats. As opposed to concrete (software) tools for working with formats that are available to end-users, integrations are embedded in their hosts and are not directly addressable by users.

Plain text Many platforms support metadata provided in plain text or lightweight markup languages by rendering them for presentation to end users. This often includes detecting URLs and converting them to HTML hyperlinks. Examples include Markdown rendering on, e.g., GitHub, GitLab, and many other platforms.

schema.org RO-Crate [37] uses schema.org [17] schemas to record and provide core metadata. Both Dataverse project and InvenioRDM offer metadata exports as schema.org JSON-LD.

CodeMeta Software Heritage [6] uses a subset⁶ of the CodeMeta vocabulary to map intrinsic metadata formats discovered in source repositories. CaltechDATA ingests CodeMeta files to create metadata records from the included metadata [29] [30]. The Astrophysics Source Code Library (ASCL) produces pre-filled CodeMeta files from its records [1] – this functionality is accessible to users through appending the URL for a record page with /codemeta.json.

Citation File Format

- Via its Github-Zenodo integration, Zenodo ingests the metadata from CITATION.cff files and uses them to populate their metadata records [36] (see also table 2 on page 16).
- Via its connector browser plugins, Zotero ingests CITATION.cff files discovered in source code repositories and saves the metadata in its internal format [11].
- JabRef can import CITATION.cff files (feature merged, currently awaiting release⁷).
- The Astrophysics Source Code Library (ASCL) produces pre-filled CITATION.cff files from its records. This functionality is accessible to users through appending the URL for a record page with /CITATION.cff [1].
- GitHub provides a template⁸ for creating new CITATION.cff files via its UI and ingests existing CITATION.cff files, extracts the metadata, converts them to a citation style and BibTeX, and provides them in a widget for end users to copy [11]. There is a feature request to implement the same for GitLab⁹.
- An extension¹⁰ to the Sphinx platform for documentation rendering ingests an existing CITATION.cff file and, converts it to different citation formats, and provides it to end users in a widget for copying (see example in [4]).
- Software Heritage can ingest CITATION.cff as intrinsic metadata format and map it (see SWH Indexer Metadata Workflow, referenced in [11]).

Zenodo JSON Via its GitHub-Zenodo integration, Zenodo ingests¹¹ .zenodo.json files and populates metadata records from the provided metadata [36].

BibTeX Usually, the metadata from $BiBT_EX$. bib files are converted into string formatted in a citation style and displayed as citations and items in the references list of LATEX based documents.

biblatex-software [7] is a reference biblatex implementation of a bibliography style extension that includes software-specific $BiBT_EX$ entries and integrates these metadata in LATEX documents.

⁶https://docs.softwareheritage.org/devel/swh-indexer/metadata-workflow.html#supported-codemeta-terms
⁷https://github.com/JabRef/jabref/issues/7945

⁸https://docs.github.com/en/repositories/managing-your-repositorys-settings-and-features/customizing-your -repository/about-citation-files

⁹https://gitlab.com/gitlab-org/gitlab/-/issues/337368

¹⁰https://www.higithub.com/citation-file-format/issue/citation-file-format/356

¹¹https://developers.zenodo.org/#add-metadata-to-your-github-repository-release

Manifest files Some or all information from manifest files is rendered on package/artifact repositories' sites for the respective package, e.g., on Maven Central, PyPI, NPMJS, Debian Packages etc.

2.4 Tooling

The following section is an attempt to gather tools available for metadata extraction, collection and durable publication. Please note: section 2.5 contains any tooling to be used as building blocks for (automatable) workflows around software depositions. These lists may not necessarily be complete.

2.4.1 Metadata

Existing toolsets for metadata may operate on different stages of metadata presence. The spectrum starts at zero prior information and requires extraction from arbitrary text files and context information. Moreover, it can be accomplished by reusing software package metadata via so called crosswalks, or even conversions between different metadata formats. Some may give users a hand to create well-structured metadata from the start.

Software Metadata Extraction Framework (SoMEF) SoMEF [15] [27] extracts data from README text files and other files that may include metadata using a neural network. It may also retrieve details from Software Development Platform text such as GitHub, using their APIs. It creates, e.g., CodeMeta JSON-LD or Turtle RDF files using The Software Ontology [14]. The projects repository status is O active.

CaltechDATA Automated Metadata Service (AMES) AMES [30] may be used to create and update scholarly output records in services like CaltechDATA, highly specific for Caltech and based on 2.4.2. For software publications a Python script to update InvenioRDM records from CodeMeta files files is in use [29]. The projects repository status is \bigcirc active.

codemeta2cff GitHub Action The codemeta2cff GitHub Action [28] provides automatic conversion from a CodeMeta files file to a Citation File Format file in a GitHub Action. The projects repository status is *suspended*.

CodeMeta Crosswalks CodeMeta Crosswalks [3] are a set of comma-separated value (CSV) files, containing two columns. Each row depicts a metadata field in CodeMeta files and a corresponding field in some other schema. While not an executable tool, these crosswalks describe a mapping with limited interoperability, as most other standards aren't as detailed. The projects repository status is **1** *inactive*.

CodeMeta Generator CodeMeta Generator [18] is a Javascript-based web UI to help you create CodeMeta files for inclusion in your software repository. The projects repository status is **1** *inactive*.

Citation File Format Converter cffconvert [41] is a Python based command line tool to transform a given Citation File Format file into other destination formats like BIBTEX files, CodeMeta files and others. It is also available as a GitHub Action. The projects repository status is \bigcirc *active*.

Citation File Format Initializer cffinit [42] is a Javascript based interactive web form to assist you in creating a new or updating an existing Citation File Format file in your browser. The projects repository status is \bigcirc active.

2.4.2 Publication repositories

Publication repositories are public catalogue containing publications of digital artifacts together with the metadata describing them. Usually, publication repositories provide landing pages for each artifact, including versions of the same object. As such, they are different from registries, that usually focus on the collection of

metadata and their presentation. They are also different from archives, that focus on long-term archival of artifacts only. Additionally there may exist differences in how records are added to publication repositories, registries and archives.

One of the main advantages of publication repositories is that they enable a combination of discovery of digital objects through their metadata, and direct access to the object artifacts themselves. HERMES focuses on publication repositories exclusively, and specifically on two publication repository software projects as deposition targets, for the reason that they represent commonly used platforms both within the Helmholtz Association and beyond: Dataverse project and InvenioRDM.

Research software is also represented in digital preservation archives (like the Software Heritage Archive [6]), catalogues and directories (like the Research Software Directory [38]). Targeting these platforms may be a future direction of development for HERMES, see also 3.4.4.

Dataverse project The Dataverse project is an open source repository software.

Its focus is currently on providing services for **Dataset** deposition, although software may be deposited as part of datasets, too. No built-in support for software metadata schemas, software licenses or propagating software metadata to PID registrars is available.

Despite versioning support for datasets, neither integrating software release versioning is available nor support for software citations as a concept and individual releases.

The Dataverse community runs a working group for software, workflow and container related topics. Its website can be found at https://swc.wgs.gdcc.io The projects repository status is O active.

InvenioRDM The InvenioRDM project has the goal to provide a turn-key research data management repository based on Invenio Framework and Zenodo. The publication of special software datasets is possible, but the standard set of metadata for the description of Invenio records is used as well as in 2.1.2.

Invenio provides versioning, DOI registration and supports multiple data types for the publication such as Publication, Poster, Presentation, Dataset, Image, Video/Audio, Software, Lesson, Physical objects or Other (list¹² taken from Zenodo). No builtin support for software metadata schemas is available at the moment.

For a software publication the use of optional webhooks can be used as introduced in Pull-based workflows. The projects repository status is \bigcirc *active*.

2.5 Workflows

Depositing scientific software to archives like Software Heritage [6] or publication repositories requires some kind of workflow, involving manual steps or automation.

Workflows may be coarsely categorized into "push" or "pull" based approaches. Both have their pros and cons, but within the context of scholarly software publications, push-based approaches have the advantage of not having to expose the source code repository to the publishing service. As making a software FAIR does not require code access [5][23], this may be beneficial to increase the number of software publications even for closed source research software.

Table 2 on page 16 provides an in-depth overview of known full-fledged workflows and tools used within custom automated jobs pertaining to software publications. Both categories of workflows are covered and analysed for their metadata extraction and publication capabilities. Please note: neither the table nor the following list of building blocks need to be complete.

Pull-based workflows may be subdivided into "harvesting" and "triggered" types.

"Harvesting" for new or changed datasets is an often used pattern within the world of text and data publications. The well-known OAI-PMH is used for inter-repository talk, while harvesting in the context of workflows is attached to pulling commits from public accessible source code repositories. Retrievals may be scheduled or kicked off by some event. To provide an example: both the Software Heritage Archive [6] and the Research Software Directory [38] use scheduled harvesting: they check for changes in source code

 $^{^{12}{}m See}$ upload_type at https://zenodo.org/schemas/deposits/records/legacyrecord.json

repositories, publishing repositories, etc. and incorporate them, which might involve updating existing metadata.

Using a webhook to "trigger" some action is a well known technique in distributed systems. Within the publication business a webhook may even trigger a harvesting action with certain parameters like a target. The GitHub-Zenodo integration¹³ is a good example for this, sending a webhook request on software package releases (tagged revisions within a source code repository) to trigger the harvest.

Push-based workflows While pull-based workflows have their advantages, in some scenarios you might want to publish your software in a more active fashion.

Push-based workflows gather metadata and/or artifacts and deposit them via some API endpoint into a service like a repository, registry or archive. They may also split certain tasks across different services, which may be harder to achieve with common pull-based workflows.

Examples for push-based workflows are even harder to find than pull-based workflow approaches. This might be due to the convenience of commonly known pull-based workflows and the not-yet popular task of software publications. Please let us know of any prototypical example we haven't listed in table 2 on page 16 yet.

Building Blocks

The following tools provide building blocks to create an automatable depositing workflow, interfacing with target repositories, registries or archives.

Zenodraft Zenodraft [39] and the corresponding GitHub action [40] may be used to draft, push and publish new deposits on Zenodo, a commonly known general purpose repository based on InvenioRDM. New and existing deposits may be enhanced with metadata via Zenodo JSON files. The project's repository status is **O** suspended.

Software Heritage Github Action SWH Github Action [8] acts like a webhook: it sends a archive request to an Software Heritage Archive API endpoint with the repository to archive given as parameter. Software Heritage Archive services take care¹⁴ of reading a CodeMeta files, Citation File Format or other metadata files via CodeMeta Crosswalks (if included) to add metadata to its archive. The project's repository status is O *suspended*.

Software Heritage Deposit Command Line Tool The CLI part of a SWORD [2] based deposition service [19] for the Software Heritage Archive may be used to actively push metadata and/or artifact ingests. It seems not to be intended for public usage but integrations with software/data repositories. The project's repository status is \bigcirc active.

Dataverse Uploader GitHub Action The Dataverse Uploader Github Action [45] enables uploading content from a source code repository into a "dataset" on a target Dataverse project installation. It allows to replace all or add to files and their metadata. The action may also publish a new dataset version afterwards. The projects repository status is \bigcirc active.

¹³https://guides.github.com/activities/citable-code

¹⁴See https://docs.softwareheritage.org/devel/swh-indexer/metadata-workflow.html

3 Concept

3.1 Overview

The coupling of software development platforms with publication repositories for automated data exchange is a first and important step for easier and automated software publications. This technical foundation also immediately raises the question as to the requirements towards a source code repository on a development platform to benefit from such automation. Current first generation tools simply copy the content of a source code repository to create or update a publication repository entry. The metadata of the publication repository entry can originate from a special file in the source code repository.

Questions addressed by HERMES that extend the status quo are:

- How to automate collation of metadata from different sources for automated publication?
- How to treat different components in a source code repository (software, documentation and data)?
- How to deal with source code repositories that contain more than one software product?
- How to deal with publication of executable software artifacts generated from the software repositories?
- How to enable closed source but FAIR software [23] for these processes?
- How to synchronize existing metadata automatically after publication?

3.2 Source code repositories

HERMES targets both GitHub and GitLab as software development platforms as they are the de facto community standard and are widely used both as public cloud services and on-premise installations. Both services offer an API for interaction with other services and, thus, provide an ideal starting point for HERMES to add on to the existing solutions.

3.2.1 Different ways of setting up software projects

A source code repository containing only one software package is an easy, common case and straightforward in publication. Integrated software documentation as part of the repository is considered a part of the software package and does not need to be treated differently.

For other cases, e.g., data alongside the source code or multiple software packages in one source code repository, HERMES allows the user to specify which parts of the repository to include in a publication.

3.3 Metadata sources

HERMES decidedly does not limit the metadata sources it works on to specific types. However, implementation follows an iterative process, with support for different types being added in stages.

- 1. Firstly, we collect structured metadata that can be tested for availability, e.g., dedicated metadata files, such as codemeta.json, CITATION.cff, LICENSE files , version control metadata , software development platform metadata (all described in Formats).
- 2. Secondly, we attempt to mine structured data that may or may not contain relevant metadata, e.g., manifest files, configuration files, etc.
- 3. Finally, we attempt to mine unstructured metadata from, e.g., plain text files.

In cases where several instances of metadata sources exist and contain overlapping – and potentially diverging – information, we follow a set of heuristics to defensively establish source precedence and avoid conflicts or bad metadata.

3.4 Scope

HERMES aims to enable software publications in publication repositories where metadata is transported from the source code repository to the publication repository. During this first iteration of the project, it interfaces with two popular publication repository software products: the Dataverse project and InvenioRDM.

3.4.1 Out of scope

The tooling developed and provided needs to be shaped in scope and size. Thus, at this stage HERMES

- does not offer license compatibility checks,
- does not resolve values from external vocabularies (e.g., WikiData, triplestores using software metadata ontologies) or other persistently identified resources (ORCID, ROR, other publications, ...),
- does not validate metadata beyond pure linting functionality,
- does not create provenance, workflow or pipeline models (but may be a part of these),
- does not search or resolve publications of (software) dependencies and
- does not run software being published to collect runtime-specific metadata.

The software and reusable workflow templates that HERMES provides does not constitute, or be provided as, a "service" (web service, REST API, SaaS, PaaS, IaaS, etc.) or other infrastructure component.

Instead, research software projects can reuse the solutions in their own software projects, e.g., by defining their own CI/CD workflows based on provided templates. This way, our outputs also have a greater potential of becoming sustainable: once they are persistently distributed, no continuous funding for HER-MES is needed to use them. Instead, the community may apply further funding as needed, e.g., for further development.

3.4.2 Expectations on users and sources

HERMES cannot clean up messy projects for users. Instead all tooling relies on the user to provide

- well-structured source code repositories
- with separated artifacts for data and software and
- with any possible legal issues resolved beforehand and appropriatly chosen licenses.

Additionally, we rely on users to supply any authentication credentials needed for workflows to run successfully. Examples include target publication repositories APIs source code platform APIs, continuous integration systems and the like.

On a side note: usage scenarios with multiple metadata sources are likely to be the norm, not the exception. Please see metadata sources for details.

3.4.3 In scope

The user receives assistance in depositing software in an automated fashion. This may be used to create publications purely with rich metadata (to be at least FAIR [5], even for closed source software) or with attached artifacts like source code, executables, etc. (to be more easily reusable). To achieve this, HERMES provides

- an extensible, configurable and automatable toolchain with capability to be executed for¹⁵
 - N software publications in
 - M target publication repositories
 - from the same origin
 - as configured by the user,
- initially harvesting and collating statically available metadata from formerly described metadata sources and
- initially targeting
 - InvenioRDM and
 - Dataverse project
- for deposits of metadata and artifacts according to curator-defined requirements
- and output of the respective metadata in a structured format (e.g., CodeMeta files) for further reuse.

 $^{^{15}\}mathrm{Please}$ take a look at figure 2 for a more visual explanation.

3.4.4 Future scopes and extensions

In the future HERMES' extensible architecture can be used to also support archives, such as Software Heritage [6], and domain and other registries such as ASCL [1], the Research Software Directory [38], etc.

3.5 Implementation outline

As discussed in In scope, we provide metadata tooling and templates to integrate this tooling in automated (CI/CD) workflows. In this section, we briefly describe the basic concepts for the implementation of this tooling.

3.5.1 Architecture

As described within scope, our implementation reuses existing computing resources by leveraging workflows on them. Figure 1 on page 17 uses a C4 component diagram to outline the overall architecture of our solution.

3.5.2 Workflow pipeline modeling

As figure 2 on page 18 outlines, HERMES implements four discrete pipelines with public interfaces for extensibility and based on existing state-of-the-art tooling where possible, namely

- 1. a metadata harvesting pipeline that
 - runs a metadata analysis to determine the concrete harvesting tools to apply to the discovered metadata sources, and
 - retrieves the existing metadata from them;
- 2. a metadata processing pipeline that
 - validates the retrieved metadata, i.e., checks for conflicting sources, and
 - merges them into a coherent set;
- 3. a metadata deposition pipeline that
 - optionally elicits metadata requirements from target publication repositories and matches the merged set against them,
 - publishes the set of metadata with or without the respective software artifacts to those target repositories, and
 - retrieves the persistent identifier for the deposition; and
- 4. a post-processing pipeline that
 - optionally updates metadata in the source repositories, e.g., with the deposition identifier,
 - notifies users of any issues that were encountered during the workflow run, and
 - passes the software and deposit metadata to any following steps in the users' CI/CD workflow.

We also provide reference implementations for commonly used continuous integration tools, such as GitLab CI, GitHub Actions and Jenkins that combine the four pipelines into a complete solution for automated publication of software with rich metadata (see also 3.5.1).

3.5.3 Adding missing functionalities to target repository software

To enable the metadata deposition pipeline described above to publish software with rich metadata, the two targeted publication repositories need to be prepared to accept metadata sets compiled in the metadata processing pipeline.

Both the Dataverse project and InvenioRDM lack some features for advanced software metadata intake and presentation. The current iteration of the HERMES project investigates and coordinates with these projects and stakeholders to add any missing functionalities upstream.

3.5.4 Templates, documentation and training resources

HERMES will safeguard the usability and sustainability of the implemented tooling by enabling the growth of a community through three main strategies: exemplary workflow templates, comprehensive documentation and the provision of training resources for end users.

We provide exemplary workflows for combinations of commonly used CI/CD systems and our target publication repository. These templates will be published under open licenses and can be adapted by end users to suit their needs.

The documentation that the project produces encompasses conceptual documentation for stakeholders (of which this paper is a starting point), technical documentation for future developers and maintainers as well as integrating parties, and documentation for end users, i.e., researchers looking to publish their software with HERMES tooling.

Furthermore, we develop training resources for end users. These resources are planned to be implemented in training curricula within the Helmholtz Association as part of the HIFIS project. Additionally, they are being made available for reuse by the wider community, and licensed under open licenses.

Tables and Figures

Metadata type	Metadata format										
Plain Text	Citant Code Men thes	There File 1 Files	anodo 150,	Bib Los files	Namites files	milieuration files	Winked Dato	Version files	Platform,	AP 15	Other
Software name	•	•	•	•	•	•	_	•	O	•	_
File system metadata	-	-	-	-	-	-	-	\bullet	lacksquare	-	•
Authorship information	\bullet	\bullet		\bullet	•	O	O	\bullet	lacksquare	lacksquare	-
Documentation reference	\bullet	\bullet	-	-	-	-	•	\bullet	-	\bullet	•
Legal and licensing info.	\bullet	\bullet	\bullet	\bullet	-	۲	-	\bullet	-	\bullet	•
Funding information	\bullet	\bullet	-	\bullet	-	-	-	\bullet	-	-	•
Domain context	\bullet	-	-	-	-	O	-	\bullet	-	O	•
Citation metrics	\bullet	-	-	-	-	-	-	\bullet	-		•
Location metadata	\bullet	\bullet		-	igodol	-	O	\bullet	•	\bullet	•
Publication dates, etc.	-	\bullet	\bullet	\bullet	\bullet	-	-	\bullet	lacksquare	\bullet	-
Categorization inform.	\bullet	\bullet	\bullet	\bullet	-	O	-	\bullet	-	lacksquare	•
Availability information	\bullet	-	-	-	-	-	-	\bullet	-	-	•
Identifiers	\bullet	\bullet	●	\bullet	•	-	-	\bullet	O	●	•
Relational metadata	\bullet	-	-	\bullet	-	\bullet	-	\bullet	O	lacksquare	-
High-level description	\bullet	\bullet	\bullet	\bullet	O	O	-	\bullet	-	lacksquare	-
Dependency information	\bullet	•	●	-	-	\bullet	\bullet	\bullet	-	lacksquare	-
Lines of code	-	-	-	-	-	-	-	\bullet	O	\bullet	•
Programming language	\bullet	-	-	-	-	\bullet	\bullet	\bullet	-	\bullet	-
Version information	\bullet	\bullet	\bullet	\bullet	O	•	igodot	ullet	•	ullet	•
Runtime requirements	\bullet	-	-	-	-	•	•	ullet	-	-	•
References	\bullet	\bullet	\bullet	\bullet	-	•	igodot	ullet	-	ullet	•
Software quality metrics	\bullet	-	-	-	-	-	\bullet	•	-	ullet	•
Development metrics	\bullet	-	-	-	-	-	-	ullet	•	ullet	•
Usage metrics	\bullet	-	-	-	-	-	-	ullet	-	ullet	•
Infrastructural metadata	ullet	-	-	-	-	-	•	ullet	O	ullet	•

 \bullet = provides type; \bullet = partially prov. type; - = does not prov. type;

Table 1: Mapping metadata types to common metadata formats.

Pull-based								Push-based					
Rescarce Software Her	Cithill Trage Arc	Gil Callect Callect	Cittlab t (Hilb Venu A TA A (V.5)	Acto to the start	XenioRDA ration	A Integral	G Citling	PI Action (2.5)	eservation SAPA SAPA	at Quality	Tool		
Status [*] Type Documentation) 6* [43]) a,b	C C	\$ [29]	S d,e	G G g,h	0 & [20]	9 [39],[40]	D • D [31]	₩ ▲ ⁱ ,[32]	j		
Extract metadata from: Zenodo JSON CodeMeta Citation File Format Other via Crosswalks Plaintext Configuration Version control system Platform API resp.	- - - - - - - -	 - -<	(♥) - (♥) (♥) (♥) - - -	 ✓ ✓ − −	✓ f	? ? ? ? ? ?	 	- - - - - - -	- - - - - - - - - - - - -	·/····································	 - -<		
Create publication w/ m.d. Mint persistent identifier Update existing metadata in Zenodo in InvenioRDM in Sw. Heritage in Other	 - -<	 - -<	(✔) (✔) - - (✔) -	- - - - -	✓ ✓ (✓) ^e −	? ? ? - -	> > > > -	 ✓ ✓ ✓ ✓ ✓ ✓ 	- - - -	 - -<	 . .<		

Note: depositing software artifacts may be part of some of these workflows. To keep the table focused on complexer metadata issues, this is left out on purpose.

Status^{*}: ◇ Active, ○ Suspended, ♥ Concept, ♥ Abandoned, ◇ Unsupported Type: ♥ Webhook, ♥ Harvesting, ▲ CI/CD-based Webhook, ♥ Script based, ▲ Web service Support: ✓ supported, (✓) indirectly supported, ? not yet known, - unsupported Sources: ■ file-based

* Using controlled vocabulary repository status

- ^a See https://archive.softwareheritage.org/save and [6]
- ^b See SWH Indexer Metadata Workflow, referenced from [11]
- ^c See section Software Heritage Github Action (2.5)
- ^d https://guides.github.com/activities/citable-code or
- https://developers.zenodo.org/#add-metadata-to-your-github-repository-release
- ^e Zenodo extends https://github.com/inveniosoftware/invenio-github (CFF since PR 89)
- $^{\rm f}$ Zenodo JSON and CFF mutually exclusive. See announcement, Zenodo PR & Zenodo Fix
- g https://github.com/zenodo/zenodo/issues/1404
- h https://gitlab.com/gitlab-org/gitlab/-/issues/25587
- ⁱ https://sara-service.org
- i https://presqt.readthedocs.io

Table 2: Existing software publication workflows and building bricks

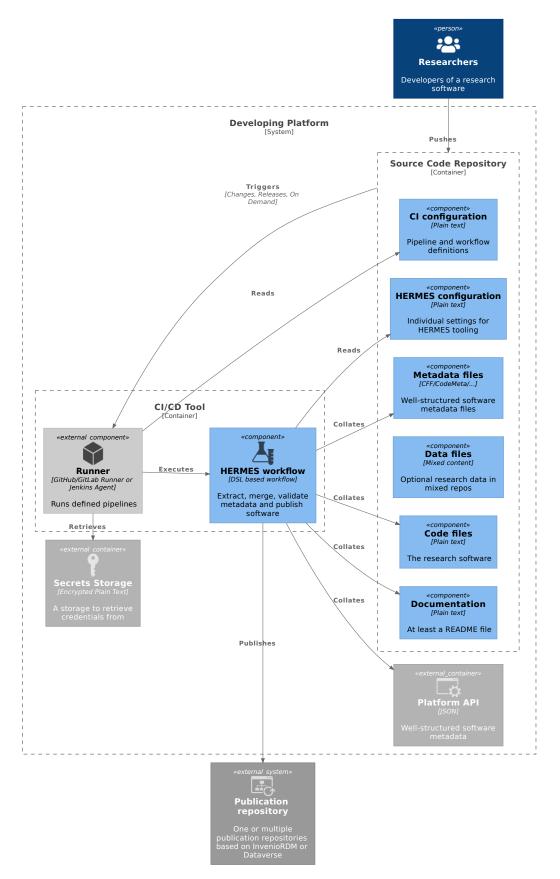


Figure 1: C4 Component architecture diagram

Outlining how the HERMES workflow relates to researchers, gets embedded in runners, collates metadata from sources and publishes in target publication repositories.

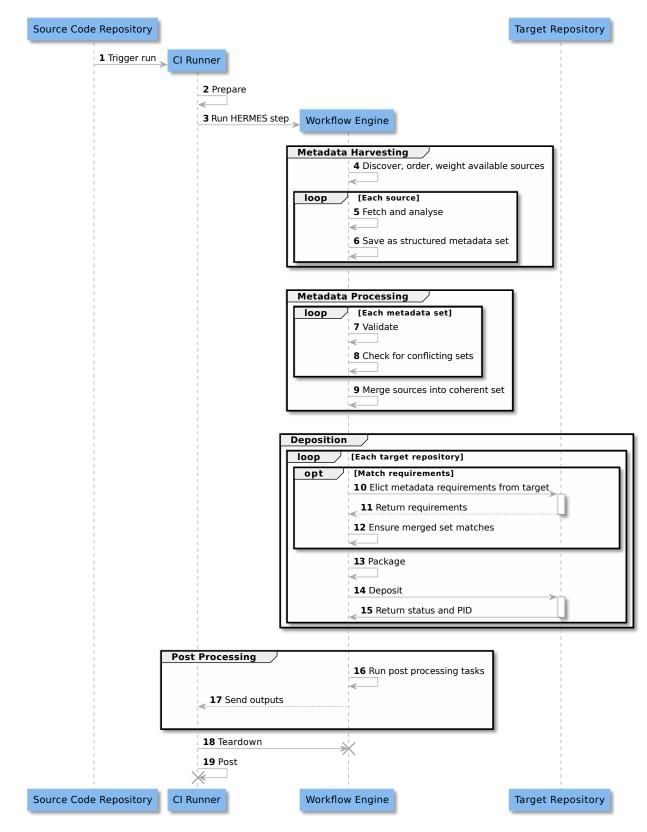


Figure 2: Sequence diagram of HERMES workflow pipelines

Simple use case (1 software, n targets) data flow, showing how HERMES workflow pipelines kick into action. Outputs of any pipeline are forwarded to the next pipeline. Both CI/CD configuration and pipelines allow for easy modifications or extensions if necessary.

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Glossary

CI/CD

Describes continuous integration/continuous deployment solutions, usually integrated in version control platforms to run automated workflows triggered by changes uploaded to the version control service. These workflows are primarily used to run automated software tests, but can also be used to run any other software automatically. Examples for CI/CD tools include GitLab CI, GitHub Actions and Jenkins automation servers. 3, 6, 12–14, 16, 18, 20

Publication Repository

A public catalogue of published artifacts that contains both the artifacts themselves as well as standardized metadata for the artifact. Each artifact is addressable with a unique identifier. 8, 14

Repository Status Controlled Vocabulary

Based on the terminology from https://www.repostatus.org, we use the different stati throughout this paper. Stati involve @ Concept, \triangleq Work In Progress, O Suspended, \forall Abandoned, O Active, Inactive, O Unsupported and I Moved. 8-10, 16

Software Development Platform text

means an online platform that supports the software development process through the combination of a version-controlled source code repository and additional tools such as issue trackers, code review tools, automation pipelines, etc. Popular examples are GitHub and GitLab. 8

Software Package

Describes a unit of functionally and/or semantically self-contained software. This meaning is opposed to the notion of package in some programming language, e.g., Java, where it is used to signify the namespace of a smaller unit, e.g., a source code file or a class. Other terms for software package include: (software) product, software (sg.), piece of software. 4, 6, 10

Source Code Repository

is a version controlled storage of directories and files usually as part of a software development platform. 5, 9, 10

Statically available metadata

Statically available software metadata can be accessed from static sources such as dedicated files or parts of files, version control systems or other forms of repositories, CI/CD contexts, file systems or platform APIs. 4, 12

Webhook

Common web technique: some software sending an HTTP POST request to a target system with the intent to trigger some kind of reaction. The request may carry a (JSON) payload, containing context, authentication, parameters and other information. 10

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