RESEARCH SOFTWARE ON WINGS

Automating software publication with rich metadata

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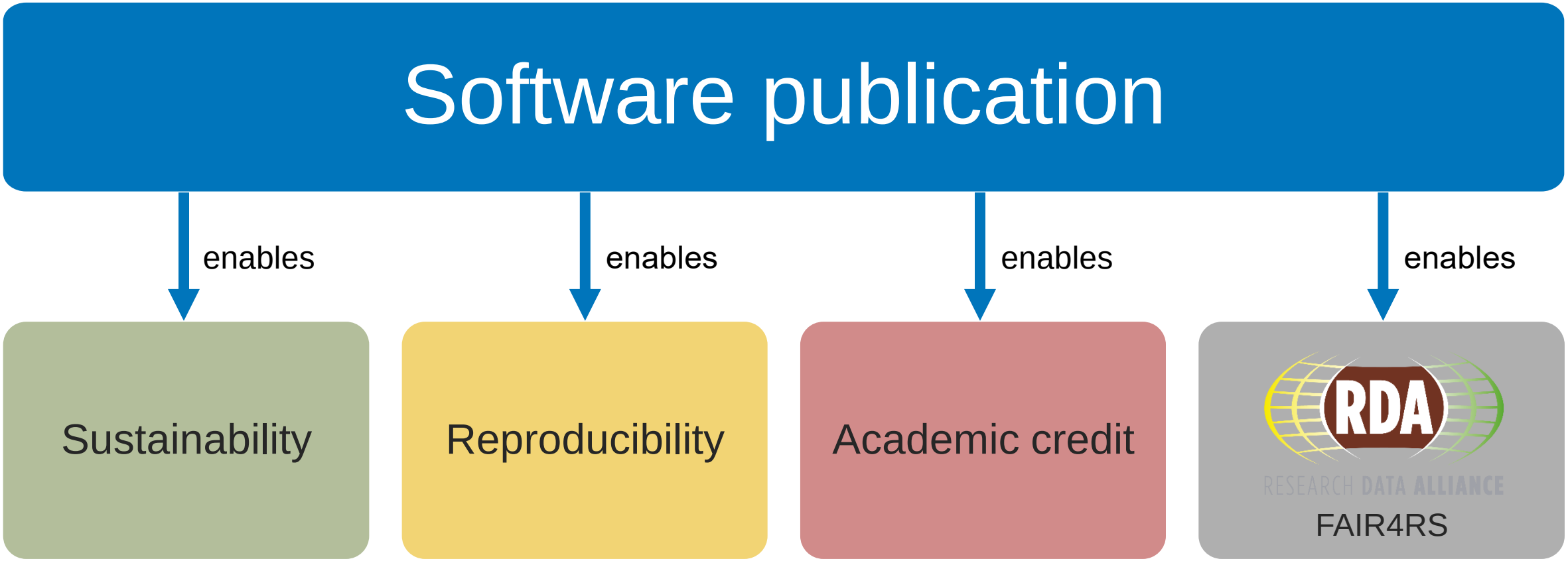
DLR

Overview

- Motivation: Software publication
- HERMES: Automating software publication with rich metadata
- Where are we now?
- Outlook

SOFTWARE PUBLICATION

Motivation: Software publication



Software publication state of the art

```python
model = getattr(spectra, spectrum_dict["type"])

if norm.unit in (u.Unit("erg"), u.Unit("erg cm-3")) and norm_type != "integral":
    raise NameError(
        "Normalisation different than 'integral' available only for 'spectrum_norm' in cm-3"
    )

# check the units of the normalisation
# cm-3 is the only one allowing more than one normalisation type
if norm.unit == u.Unit("cm-3"):
    if norm_type == "differential":
        final_model = model(norm, **spectrum_dict["parameters"])
    elif norm_type == "gamma=1":
        final_model = model.from_norm_at_gamma_1(
```

```json
{
    "@context": "https://doi.org/10.5063/schema/codemeta-2.0",
    "@type": "SoftwareSourceCode",
    "license": "https://spdx.org/licenses/BSD-3-Clause",
    "codeRepository": "https://github.com/cosimoNigro/agnpy",
    "contIntegration": "https://github.com/cosimoNigro/agnpy/actions",
    "dateCreated": "2019-12-17",
    "datePublished": "2022-01-31",
    "dateModified": "2021-08-02",
    "downloadUrl": "https://github.com/cosimoNigro/agnpy/releases/tag/v0.1.6",
    "issueTracker": "https://github.com/cosimoNigro/agnpy/issues",
    "name": "agnpy",
    "version": "0.1.8",
    "identifier": "10.5281/zenodo.4055175",
    "description": "agnpy is a python package focusing on the computation of the
    "applicationCategory": "astrophysics",
    "funding": "ESCAPE EU H2020 824064",
    "developmentStatus": "active",
    "isPartOf": "https://www.astropy.org/affiliated/#affiliated-packages",
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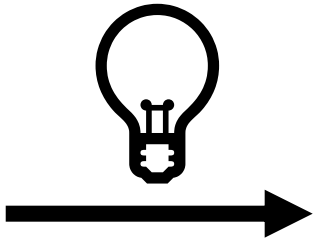
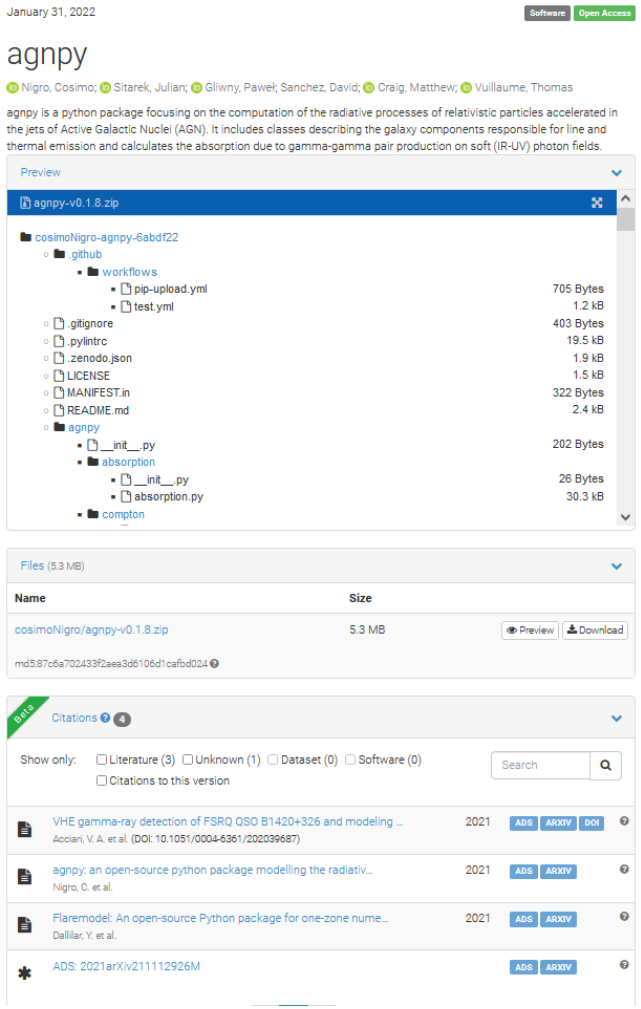


Software metadata + (software artifacts)

PID + landing page (metadata)



HERMES: Automating software publication

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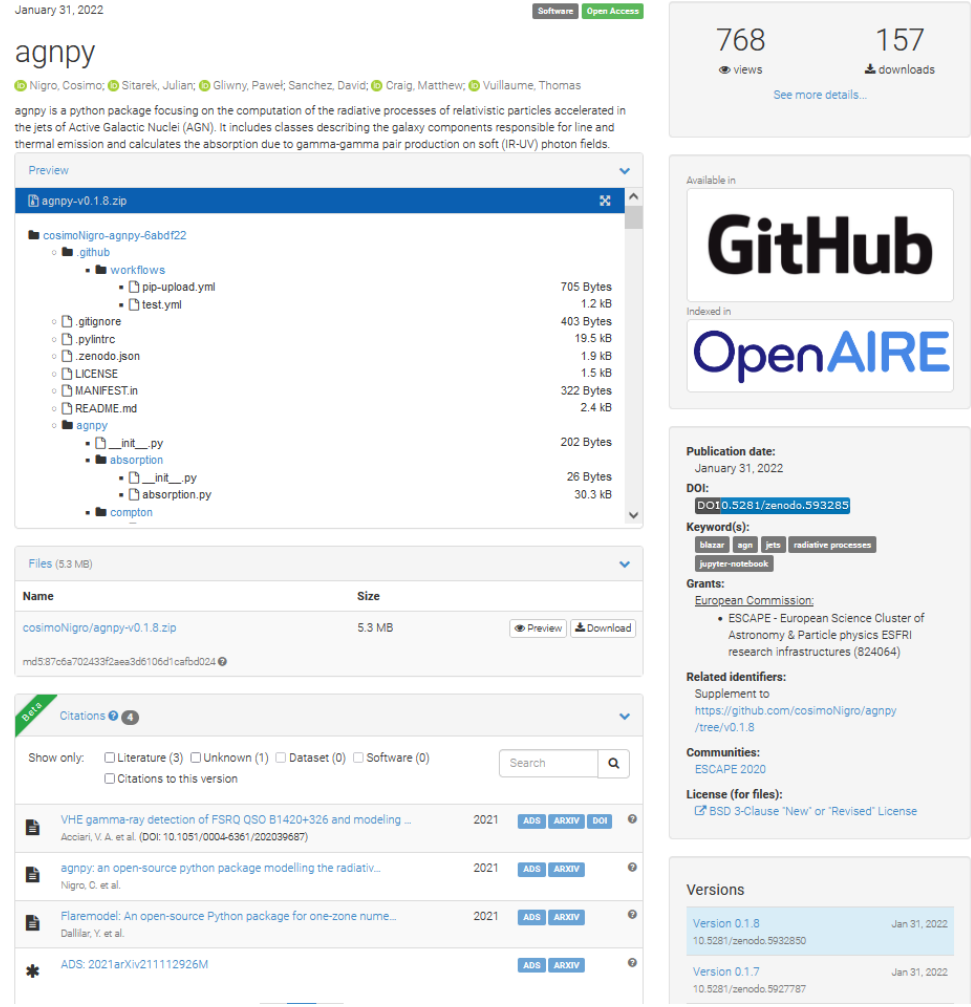
HERMES



HERMES PROJECT

HERMES: Project

HERMES

HMC | HELMHOLTZ METADATA COLLABORATION

DLR

JÜLICH Forschungszentrum

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

- 07/2021 – 06/2023
- Aim: Support RSEs in automatedly publishing their software with rich metadata

Software publications with rich metadata

State of the art, automated workflows and HERMES concept

Druskat, Stephan [1,*], Bertuch, Oliver [2], Juckeland, Guido [3], Knodel, Oliver [3], and Schlauch, Tobias [1]

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January 25, 2022

Version 1

Abstract

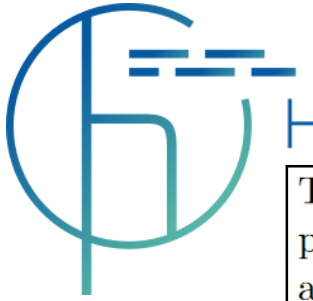
To satisfy the principles of FAIR software, software sustainability and software citation, research software must be formally published. Publication repositories make this possible and provide published software versions with unique and persistent identifiers. However, software publication is still a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

[arXiv:2201.09015 | PubPeer] | software-metadata.pub

HERMES: Scope



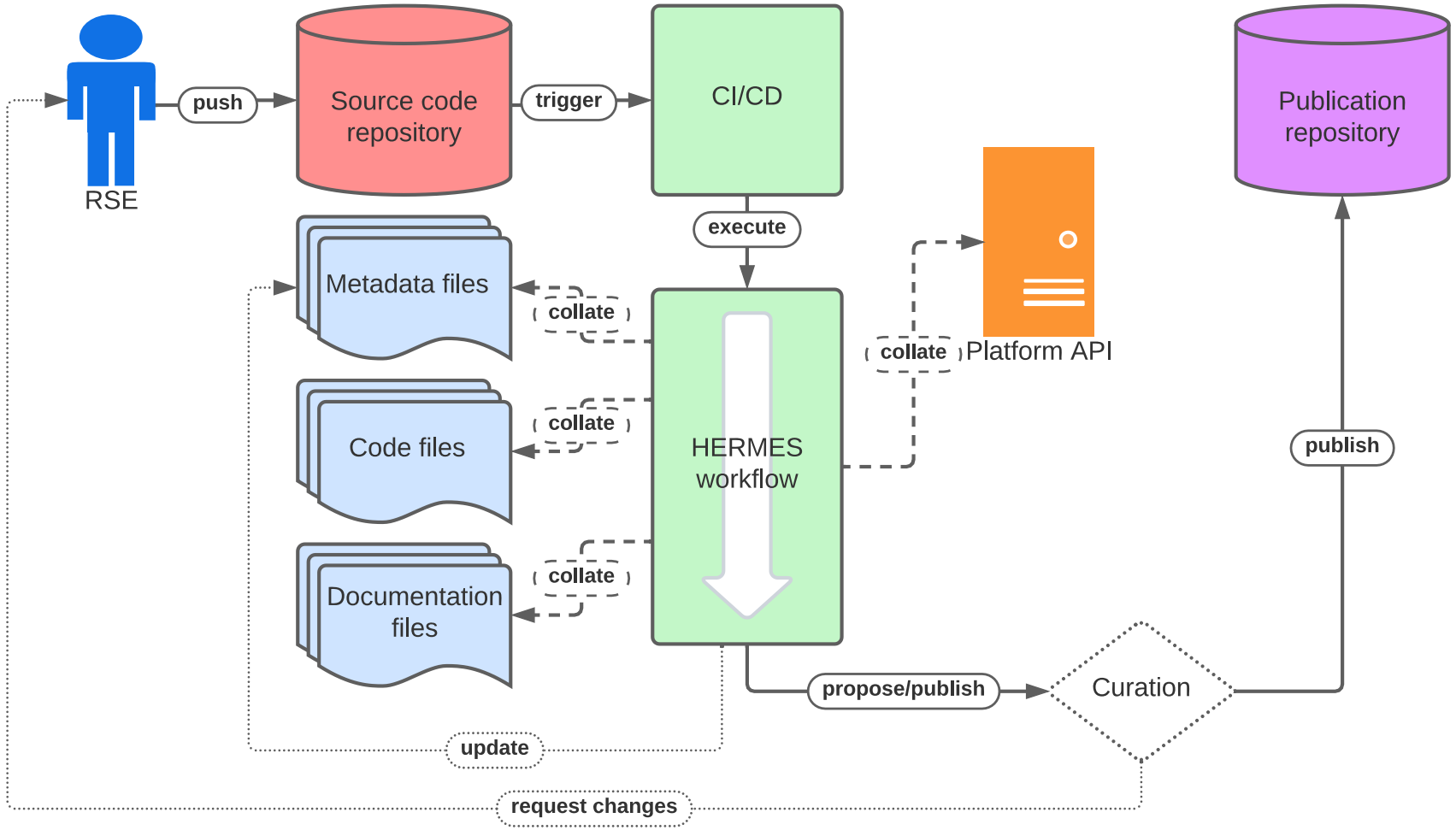
HERMES

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

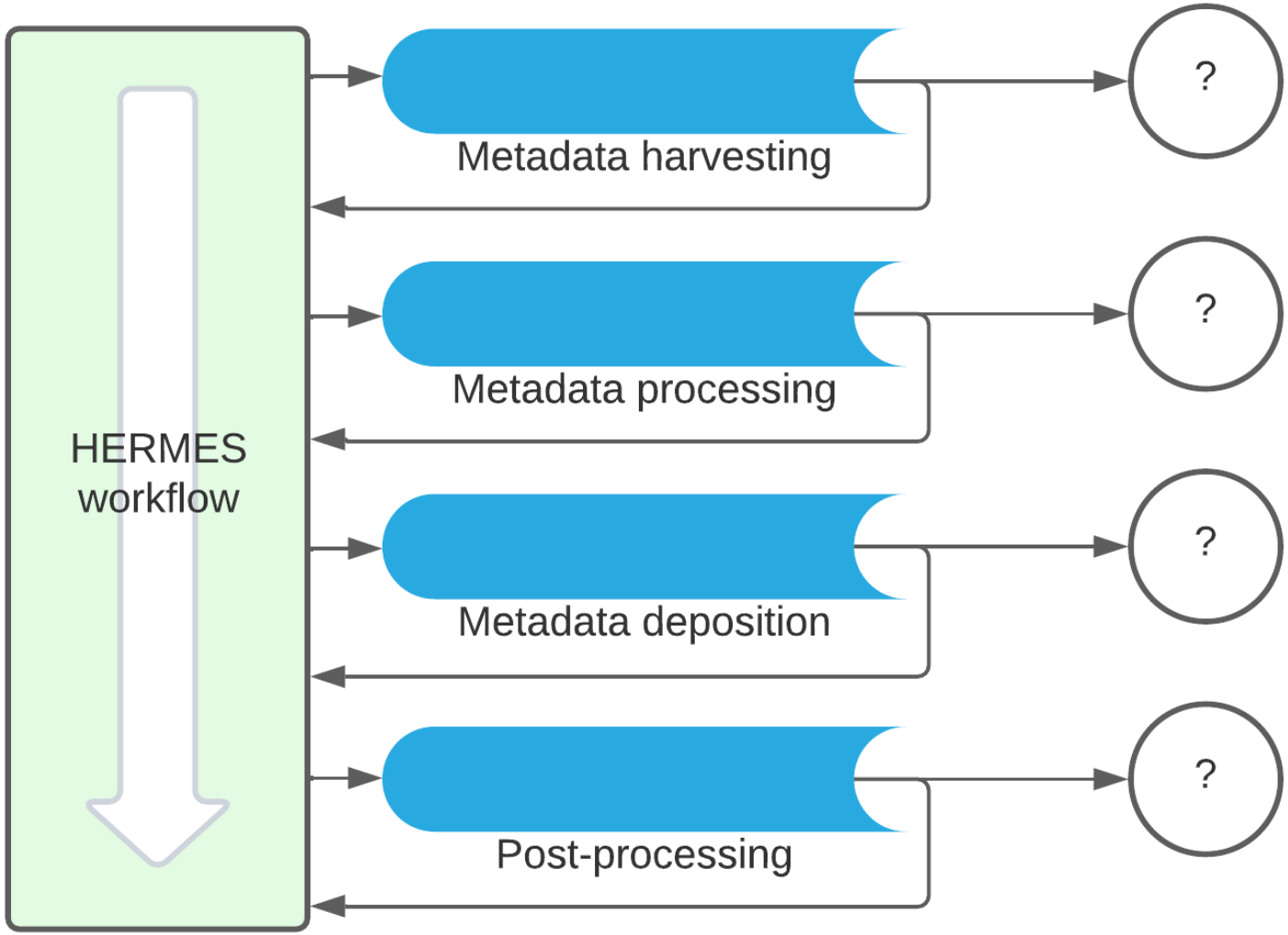
- an extensible, configurable and automatable toolchain with capability to be executed for[15]
  - N software publications in
  - M target publication repositories
  - from the same origin
  - as configured by the user,
- initially harvesting and collating statically available metadata from formerly 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.

Druskat, S., Bertuch, O., Juckeland, G., Knodel, O., & Schlauch, T. (2022). Software publications with rich metadata: state of the art, automated workflows and HERMES concept. ArXiv, abs/2201.09015.

HERMES: Concept



HERMES: Workflow pipelines



HERMES: Metadata

- **Metadata**
  - Differences in generation, scope, mode, aspects
  - Generic software metadata vs. software-specific metadata
- **Metadata formats**
  - Metadata files, snippets, third-party systems, API responses
  - Structured vs. unstructured
- **Sources**
  - Collectable structured metadata
  - (Metadata from minable structured data)
  - (Metadata from minable unstructured data)

HERMES: Outputs

- **Software**
  - Software for software publication workflow automation (workflow runner + modular pipelines)
- **CI templates**
  - GitLab CI, GitHub Actions, Jenkins, Travis CI
- **Improved research software-readiness in publication repositories**
  - Position paper “research software-ready repositories”
  - Respective contributions to Dataverse + InvenioRDM (data models, UI)
- **Training materials**
  - Adaption of open Helmholtz training materials (HIFIS) to include workflow usage
- **Project website**
  - One-stop shop for information and documentation
- **Policy proposals**
  - Proposals for updates to policies/guidelines at Helmholtz and cross-institutional

PROJECT PROGRESS

HERMES: Roadmap

Concept

- Concept paper ☑/(⚙)
- Requirements analysis ☑/⚙

Implementation

- HERMES tools ⚙
- Dataverse / InvenioRDM data model + UI ⚙
- Project website ☑/⚙

Distribution

- see outputs ⚙

HERMES: Where are we now?

- **Community outreach and consultation**
  - Stakeholders: repository projects, related metadata tools, infrastructure providers
  - Users: RSEs, IT departments, computing centres ← **you**

Test-drive & have your say at our **workshop** „Cooking FAIR research software with HERMES":
Wednesday, 7 Sep, **09:00-12:30**, room 2.16

- **Workflow implementation**
  - Harvesting: Citation File Format, CodeMeta, git metadata
  - Processing: `# TODO` (unified data model)
  - Curation: `# TODO` (user feedback via logs)
  - Deposition, post-processing: `# TODO` (CodeMeta files)

- **Research software-ready repositories**
  - Dataverse, InvenioRDM

OUTLOOK

HERMES: Outlook

- **Project ends:**
  - Automated research software publication with rich metadata
- **Potential future work:**
  - New target repositories:
    - SURESOFT (TU Braunschweig)!
    - Helmholtz research software directory?
    - NFDI publication repositories?
  - New metadata types via extended metadata mining
  - Curation UI
  - Support for research software KPIs

Thanks!

Get in touch …

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HERMES at RSECon

Stephan Druskat

Michael Meinel

Oliver Bertuch

Jeffrey Kelling

Oliver Knodel

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