

HERMES: RESEARCH SOFTWARE ON WINGS

Automating software publication with rich metadata



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OVERVIEW

- Software publication
- Project details



... AND
SOFTWARE!

SOFTWARE PUBLICATION

SOFTWARE PUBLICATION

Software publication

enables

Sustainability

enables

Reproducibility

enables

Academic credit

enables

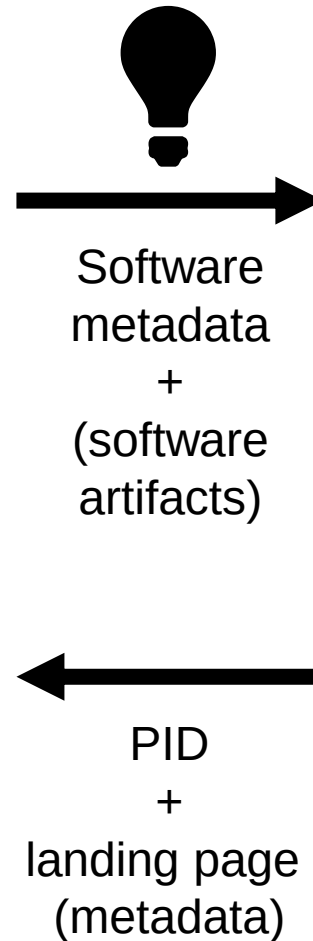


SOFTWARE PUBLICATION: STATE OF THE ART

```
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(
            norm, **spectrum_dict["parameters"]
        )
    else:
        raise ValueError(f"Norm type {norm_type} not supported")
else:
    {"@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",
```



January 31, 2022 Software Open Access

agnpy

Nigro, Cosimo; Sitarek, Julian; Gliwny, Pawel; Sanchez, David; Craig, Matthew; Vuillaume, Thomas

agnpy is a python package focusing on the computation of the radiative processes of relativistic particles accelerated in the jets of Active Galactic Nuclei (AGN). It includes classes describing the galaxy components responsible for line and thermal emission and calculates the absorption due to gamma-gamma pair production on soft (IR-UV) photon fields.

Preview

agnpy-v0.1.8.zip

- cosimoNigro-agnpy-6abd722
 - github
 - workflows
 - pip-upload.yml 705 Bytes 1.2 kB
 - test.yml 403 Bytes 19.5 kB
 - gltignore 1.9 kB
 - pylintrc 1.5 kB
 - zenodo.json 322 Bytes 2.4 kB
 - LICENSE
 - MANIFEST.in
 - README.md
 - agnpy
 - __init__.py 202 Bytes
 - absorption
 - __init__.py 26 Bytes
 - absorption.py 30.3 kB
 - compton

Files (5.3 MB)

Name	Size	Preview	Download
cosimoNigro/agnpy-v0.1.8.zip	5.3 MB		
md5:87c6a702439f2aas3d6106d1cafd0204			

Citations 4

Show only: ☐ Literature (3) ☐ Unknown (1) ☐ Dataset (0) ☐ Software (0) ☐ Citations to this version

VHE gamma-ray detection of FSRQ QSO B1420+326 and modeling ...
Acciari, V. A. et al. (DOI: 10.1051/0004-6361/202039687) 2021 ADS ARXIV DOI

agnpy: an open-source python package modelling the radiativ...
Nigro, C. et al. 2021 ADS ARXIV

Flaremodel: An open-source Python package for one-zone nume...
Dallier, Y. et al. 2021 ADS ARXIV

ADS: 2021arXiv21112926M ADS ARXIV

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Available in

GitHub

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Publication date:
January 31, 2022

DOI:
[DOI:10.5281/zenodo.593285](https://doi.org/10.5281/zenodo.593285)

Keyword(s):
blazar agn jets radiative processes
jupyter-notebook

Grants:
[European Commission](#)

- ESCAPE - European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures (824064)

Related identifiers:
Supplement to <https://github.com/cosimoNigro/agnpy/tree/v0.1.8>

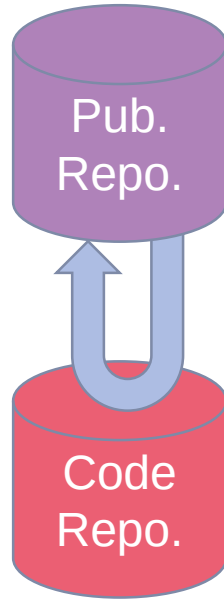
Communities:
ESCAPE 2020

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Versions

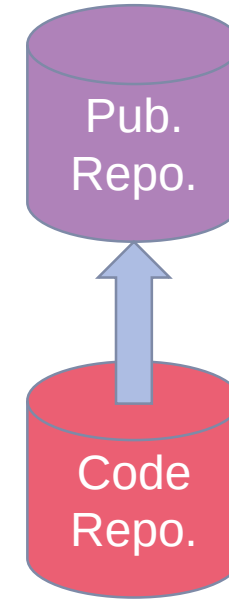
Version	10.5281/zenodo.5932850	Jan 31, 2022
Version 0.1.8		
Version 0.1.7	10.5281/zenodo.5927787	Jan 31, 2022

SOFTWARE PUBLICATION: STATE OF THE ART II



Pull-based workflows

- Code & metadata must be accessible
- Less control over extracted metadata
- Zenodo (and SWH) most prominent



Push-based workflows

- Works for all sw. types (CSS, ISS & OSS)
- Complete control over metadata
- Central service and/or decentral scripting



PROJECT DETAILS

The logo for HERMES, featuring a stylized 'H' inside a circle, followed by the word 'HERMES' in a blue, sans-serif font.

- arXiv:2201.09015v1 [cs.SE] 22 Jan 2022

Software publications with rich metadata

State of the art, automated workflows and HERMES concept

Druskat, Stephan , Bertuch, Oliver , Juckeland, Guido ,
Knodel, Oliver , and Schlauch, Tobias 

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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 advances the state of the art in research software publication.

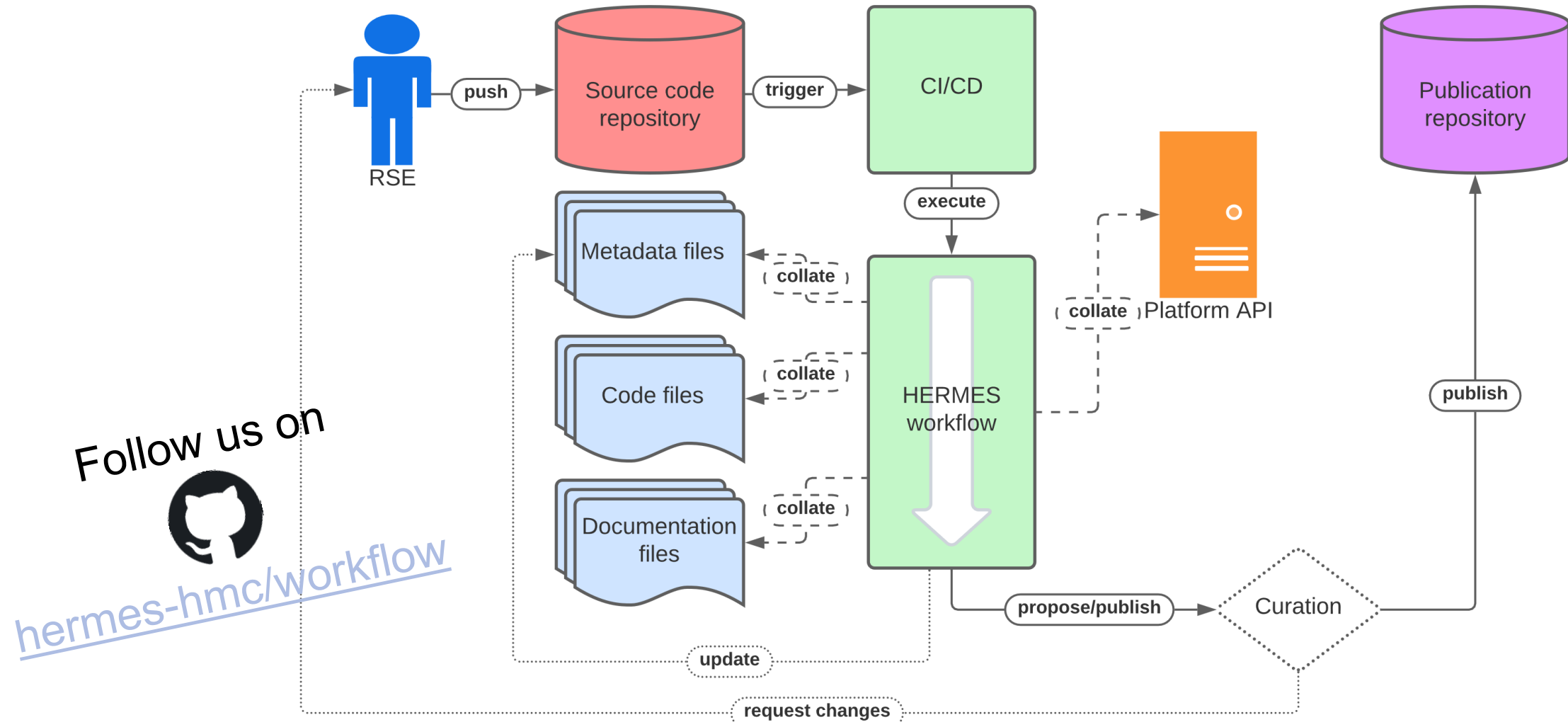
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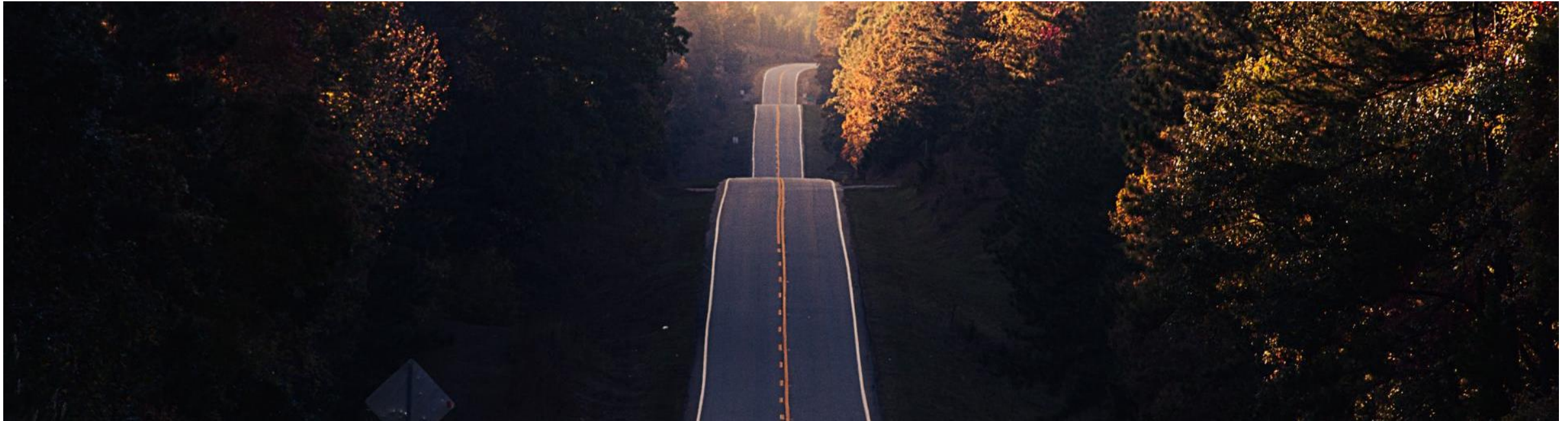


HERMES: OUTPUTS (FOR THIS ITERATION)

- **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

HERMES: CONCEPT





THANK YOU

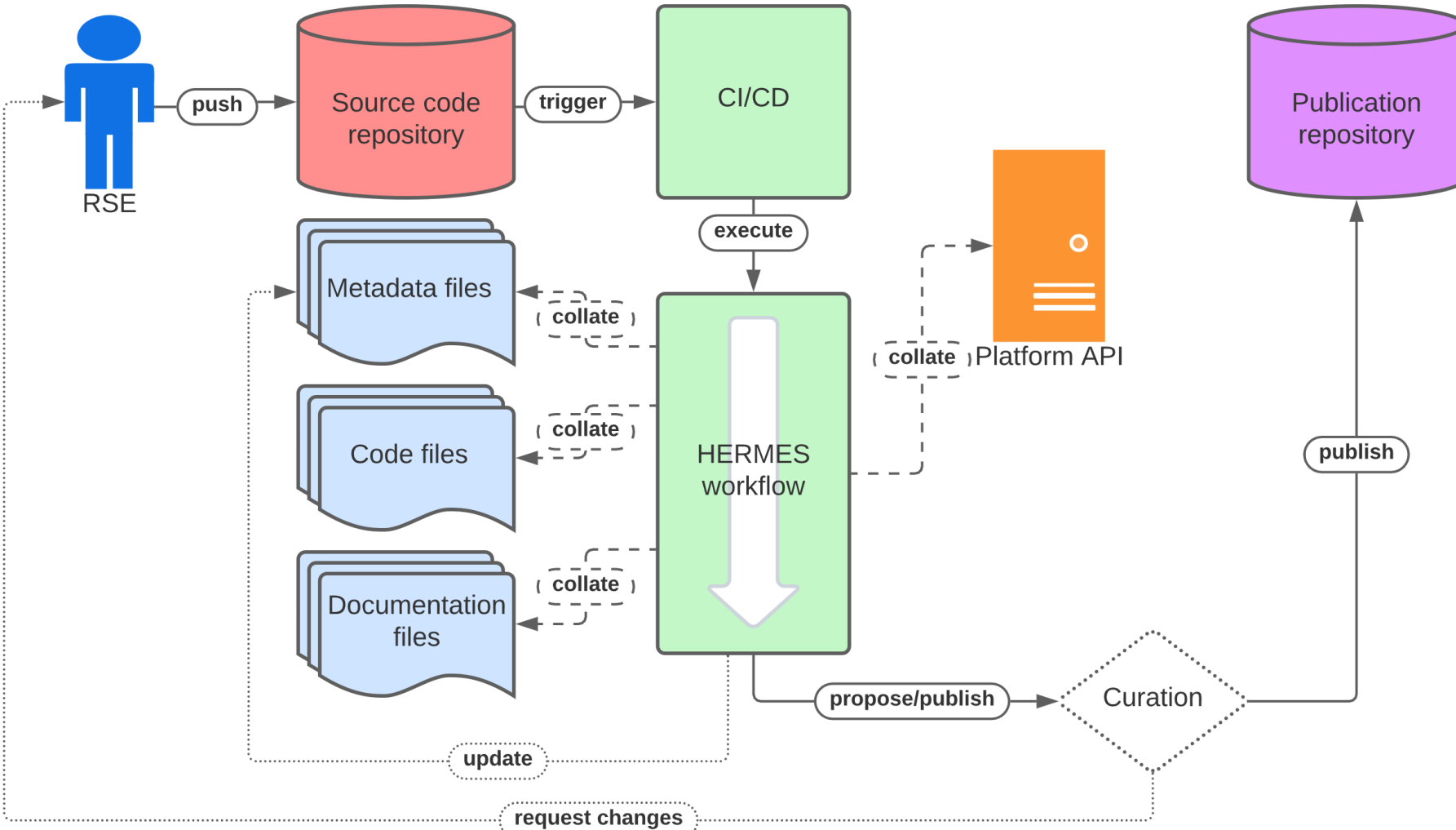
TEAM@SOFTWARE-METADATA.PUB

[GO.FZJ.DE/OBERTUCH](https://go.fzj.de/obertuch)

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

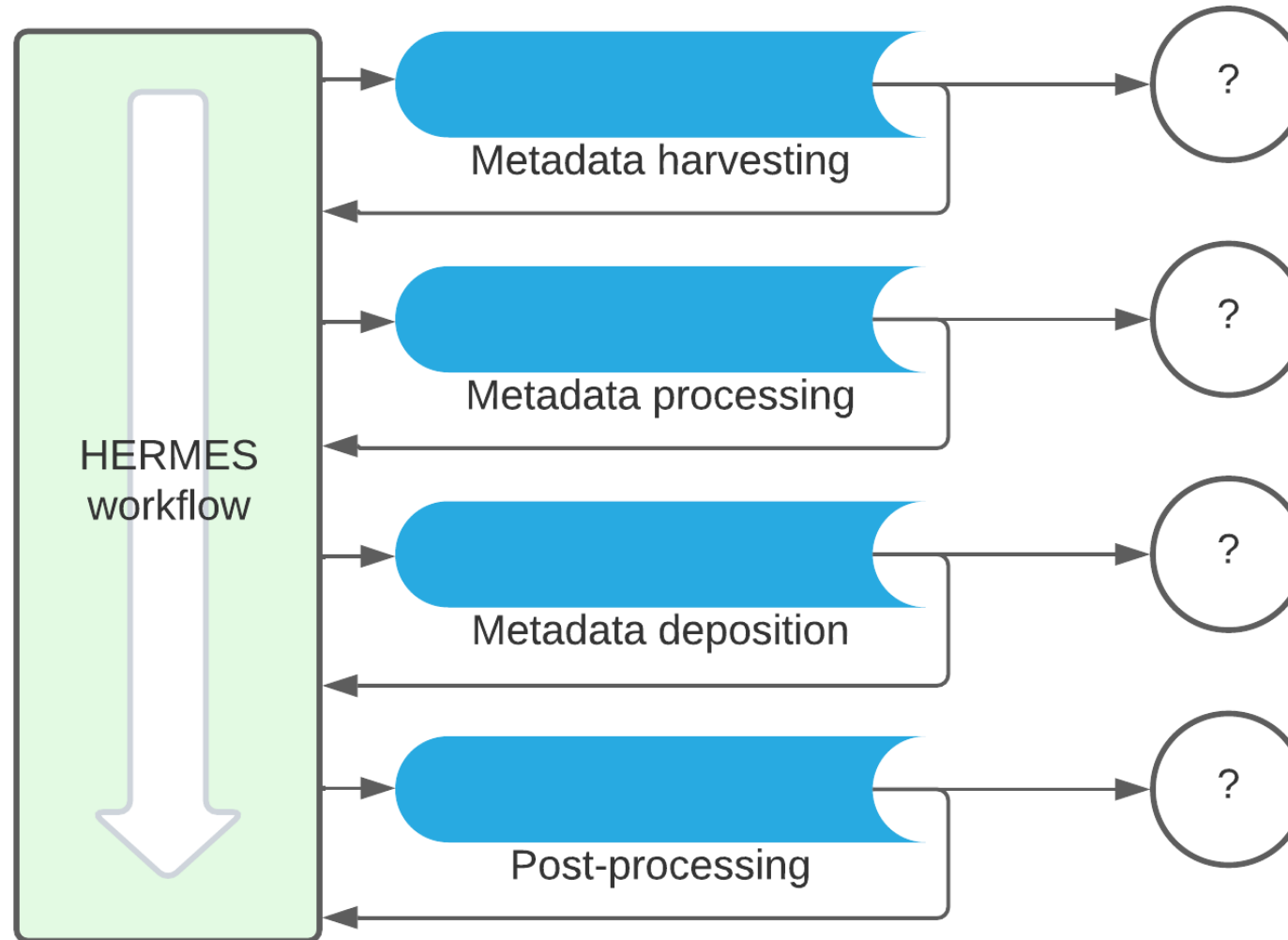
HERMES: STATUS



Where we are:

- Harvesting:
Citation File Format,
CodeMeta, Git metadata
- Processing:
#TODO (unified data model)
- Curation/Deposition:
#TODO
(user feedback via logs)
- Post-processing:
#TODO (CodeMeta files)

HERMES: PIPELINE



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: ARCHITECTURE

