Automated FAIR4RS: Software publication with HERMES

Stephan Druskat, Michael Meinel, Tobias Schlauch
Deutsches Zentrum für Luft- und Raumfahrt

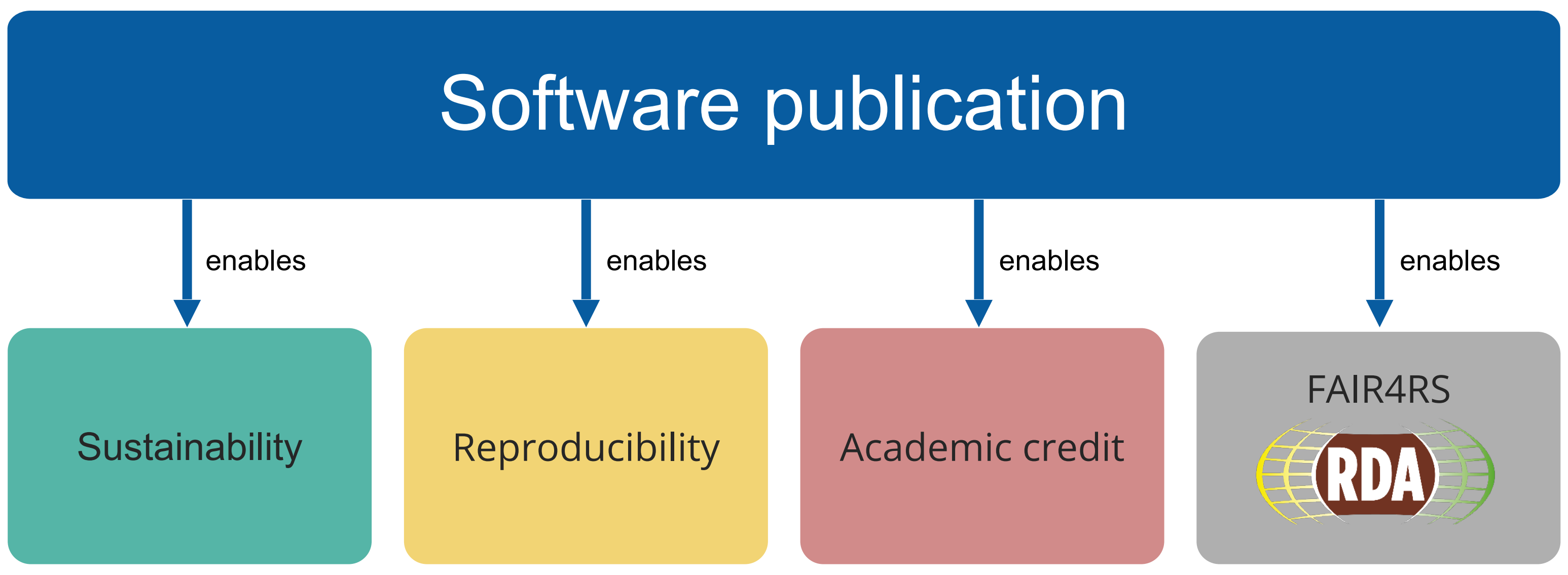
Jeffrey Kelling, Oliver Knodel, Guido Juckeland
Helmholtz-Zentrum Dresden-Rossendorf

Oliver Bertuch
Forschungszentrum Jülich

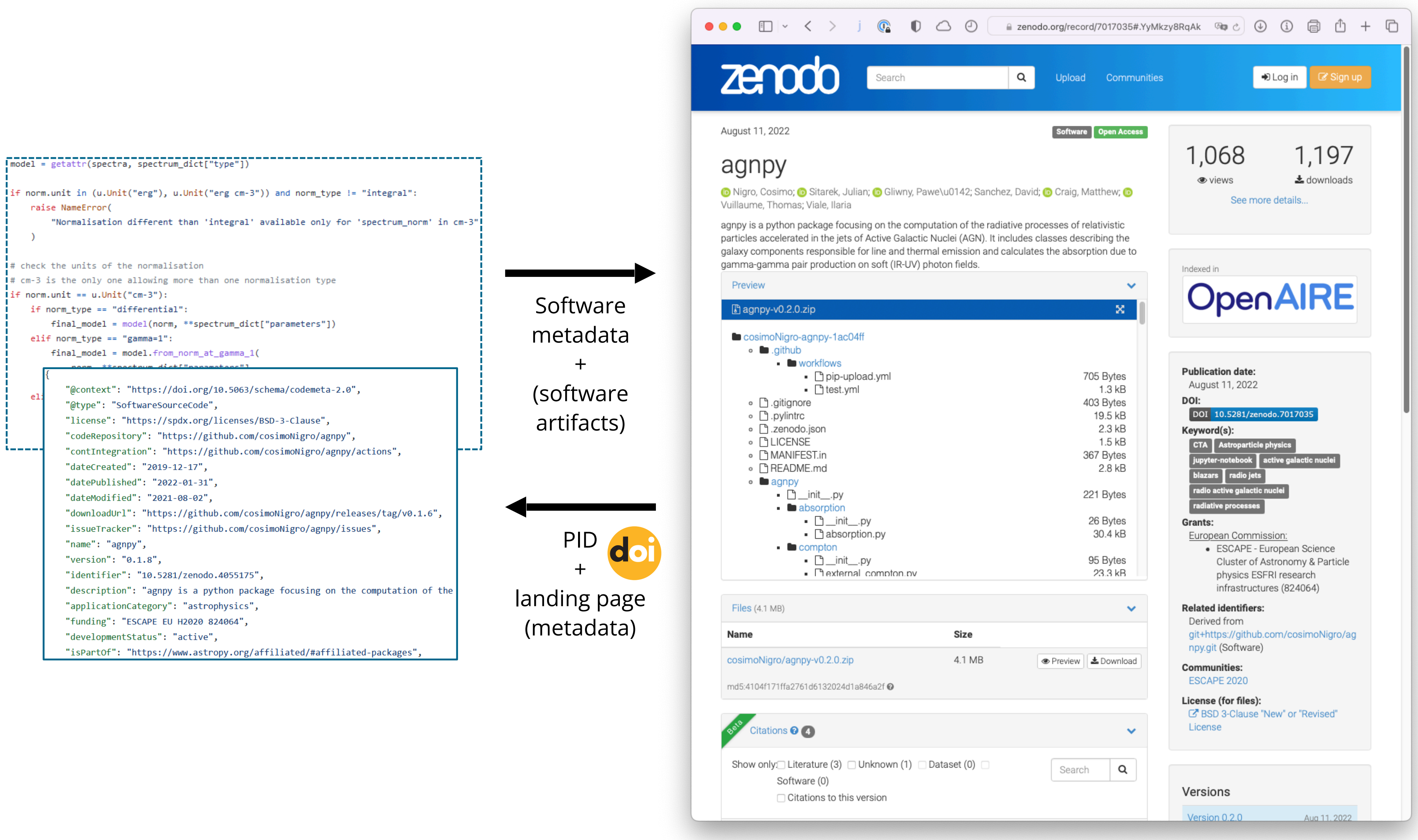
project.software-metadata.pub
github.com/hermes-hmc
team@software-metadata.pub

> To satisfy the principles of FAIR research 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 and impedes promoting software to first class research citizenship.

RESEARCH SOFTWARE READY



The 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(
```

```
{
  "@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",
```

Software metadata + (software artifacts)
PID + landing page (metadata)
zenodo.org/record/7017035#.YyMkzy8RqAk
zenodo
Search
Upload
Communities
Log in
Sign up

August 11, 2022 · Software · Open Access

agnpy

Nigro, Cosimo; Sitarek, Julian; Gliwny, Pawe\u0142; Sanchez, David; Craig, Matthew; Vuillaume, Thomas; Viale, Ilaria

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-v0.2.0.zip

```
cosimoNigro-agnpy-1ac04ff
  .github
    workflows
      pip-upload.yml          705 Bytes
      test.yml                   1.3 kB
  .gitignore                  403 Bytes
  .pylintrc                    19.5 kB
  .zenodo.json                  2.3 kB
  LICENSE                       1.5 kB
  MANIFEST.in                 367 Bytes
  README.md                     2.8 kB
  agnpy
    __init__.py               221 Bytes
    absorption
      __init__.py              26 Bytes
      absorption.py            30.4 kB
    compton
      __init__.py              95 Bytes
      external_compton.py      23.3 kB
```

Files (4.1 MB)

Name	Size	
cosimoNigro/agnpy-v0.2.0.zip	4.1 MB	Preview Download

md5:4104f171ffa2761d6132024d1a846a2f

Beta Citations 4

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

1,068 views · 1,197 downloads
See more details...

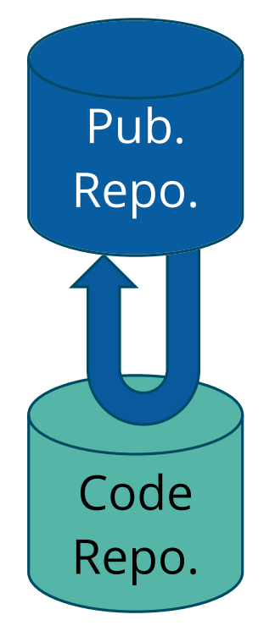
Indexed in OpenAIRE

Publication date: August 11, 2022
DOI: 10.5281/zenodo.7017035
Keyword(s): CTA, Astroparticle physics, jupyter-notebook, active galactic nuclei, blazars, radio jets, radio active galactic nuclei, radiative processes
Grants: European Commission:
- ESCAPE - European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures (824064)

Related identifiers: Derived from git+https://github.com/cosimoNigro/agnpy.git (Software)
Communities: ESCAPE 2020
License (for files): BSD 3-Clause "New" or "Revised" License

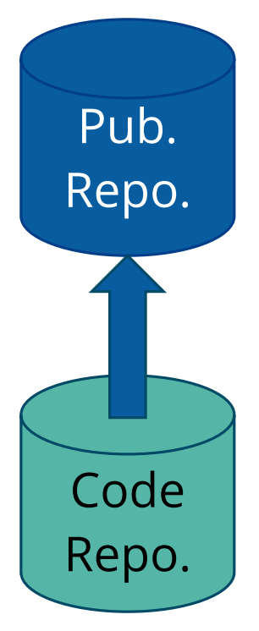
Versions
Version 0.2.0 Aug 11, 2022

Pull-based workflows



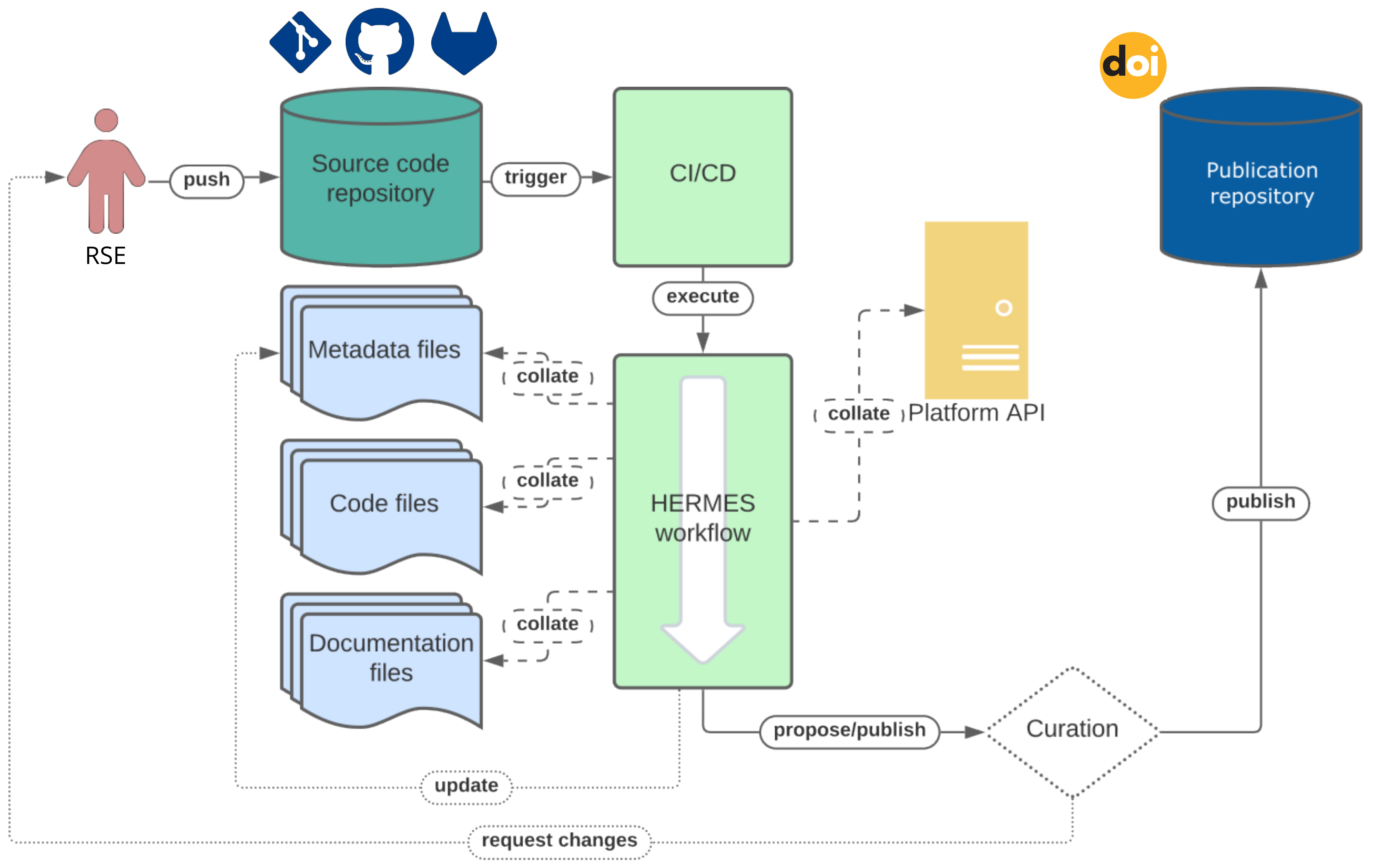
- ➖ Code & metadata must be accessible and properly formatted
- ➖ Less control over extracted metadata
- ➕ Most prominent examples: Zenodo (and SWH)

Push-based workflows



- ➕ Works for all types of software (closed, restricted, embargoed, open source)
- ➕ Complete control over metadata
- ➖ Not many examples or standardised procedures

Simplified Overview of the HERMES Workflow



Target Repositories

INVENIO RDM

The Dataverse® Project

Where we are

✓ Harvesting:
#Done: Citation File Format, CodeMeta, Git metadata

● Processing:
#ToDo: Unified data model

✗ Curation/Deposition:
#ToDo: Deposition pipelines and user feedback via logs

● Post-processing:
#ToDo: (CodeMeta files)

✓ = Present | ● = Partially | ✗ = ToDo

DLR · HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF · JÜLICH Forschungszentrum

Funded by:
<HMC> HELMHOLTZ METADATA COLLABORATION
HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES