

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:
        final_model = model

el
{
    "@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)

January 31, 2022 Software Open Access

agnpy

Nigro, Cosimo; Sitarek, Julian; Gliwny, Paweł; 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
 - test.yml 1.2 kB
 - gignore 403 Bytes
 - pylintrc 19.5 kB
 - zenodo.json 1.9 kB
 - LICENSE 1.5 kB
 - MANIFEST.in 322 Bytes
 - README.md 2.4 kB
 - 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		
md5:587c5a702438f2aa33d5106d1cafb0204			

Citations 1

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...
Dall'ier, Y. et al. 2021 ADS ARXIV
- ADS: 2021arXiv211112926M ADS ARXIV

768 157

views downloads

[See more details...](#)

Available in

GitHub

Indexed in

OpenAIRE

Publication date:
January 31, 2022

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>

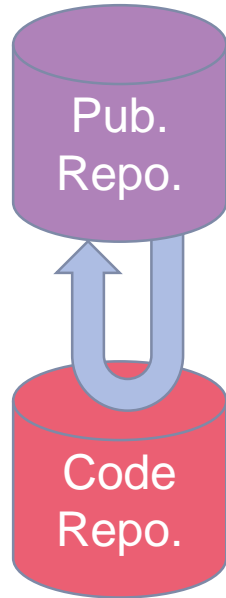
Communities:
ESCAPE 2020

License (for files):
[BSD 3-Clause 'New' or 'Revised' License](#)

Versions

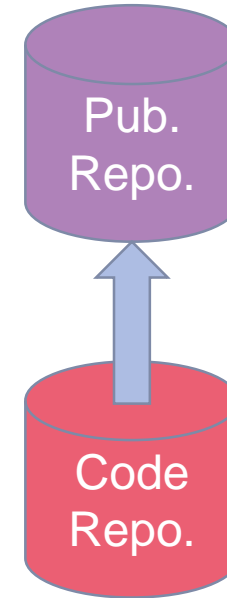
Version	Date
Version 0.1.8 10.5281/zenodo.5932850	Jan 31, 2022
Version 0.1.7 10.5281/zenodo.5927787	Jan 31, 2022

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

HERMES: PROJECT



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



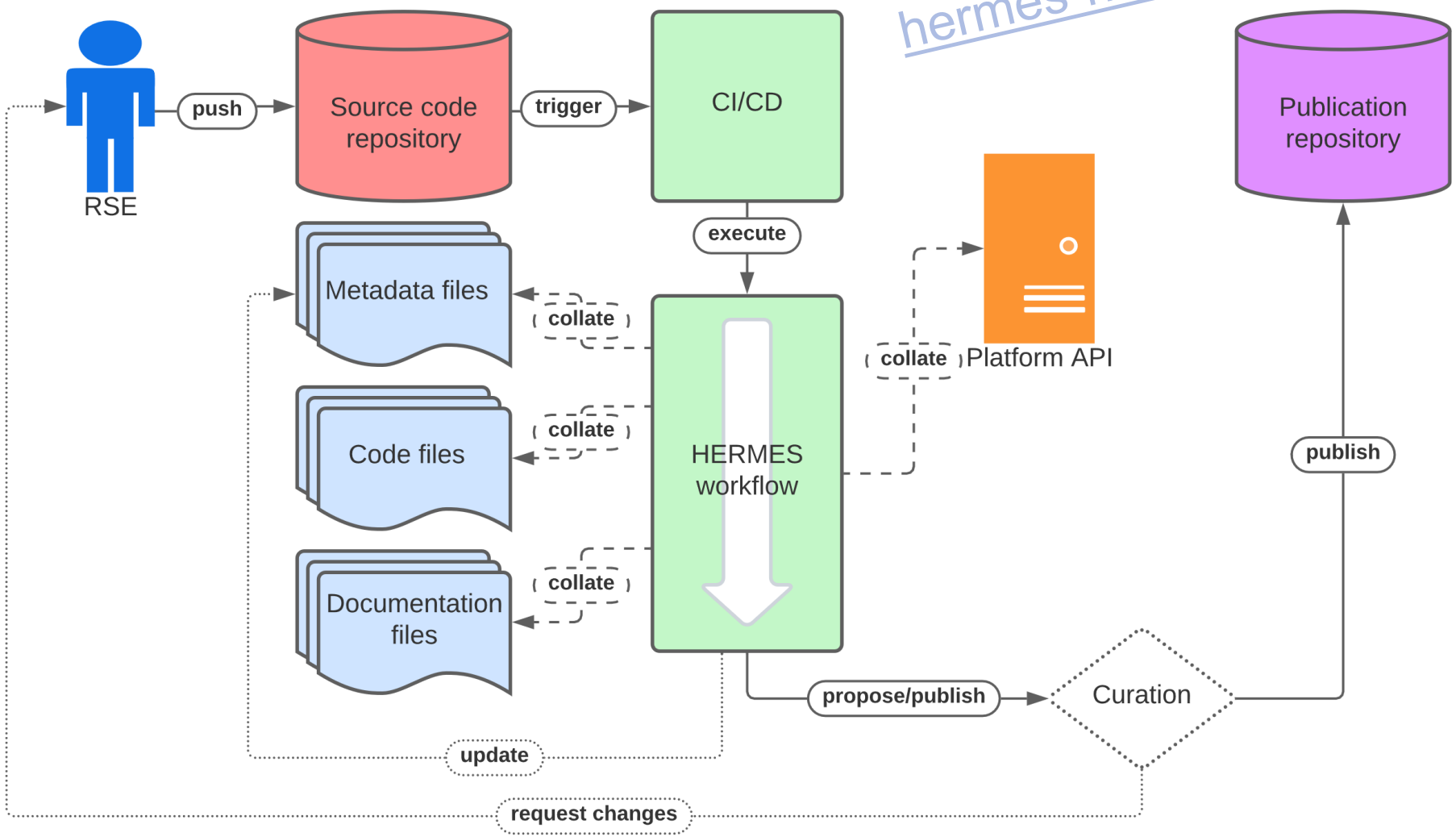
[[arXiv:2201.09015](https://arxiv.org/abs/2201.09015) | [PubPeer](https://pubpeer.com/public?id/220109015)] | software-metadata.pub

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 I


Follow us on 
[hermes-hmc/workflow](https://github.com/hermes-hmc/workflow)

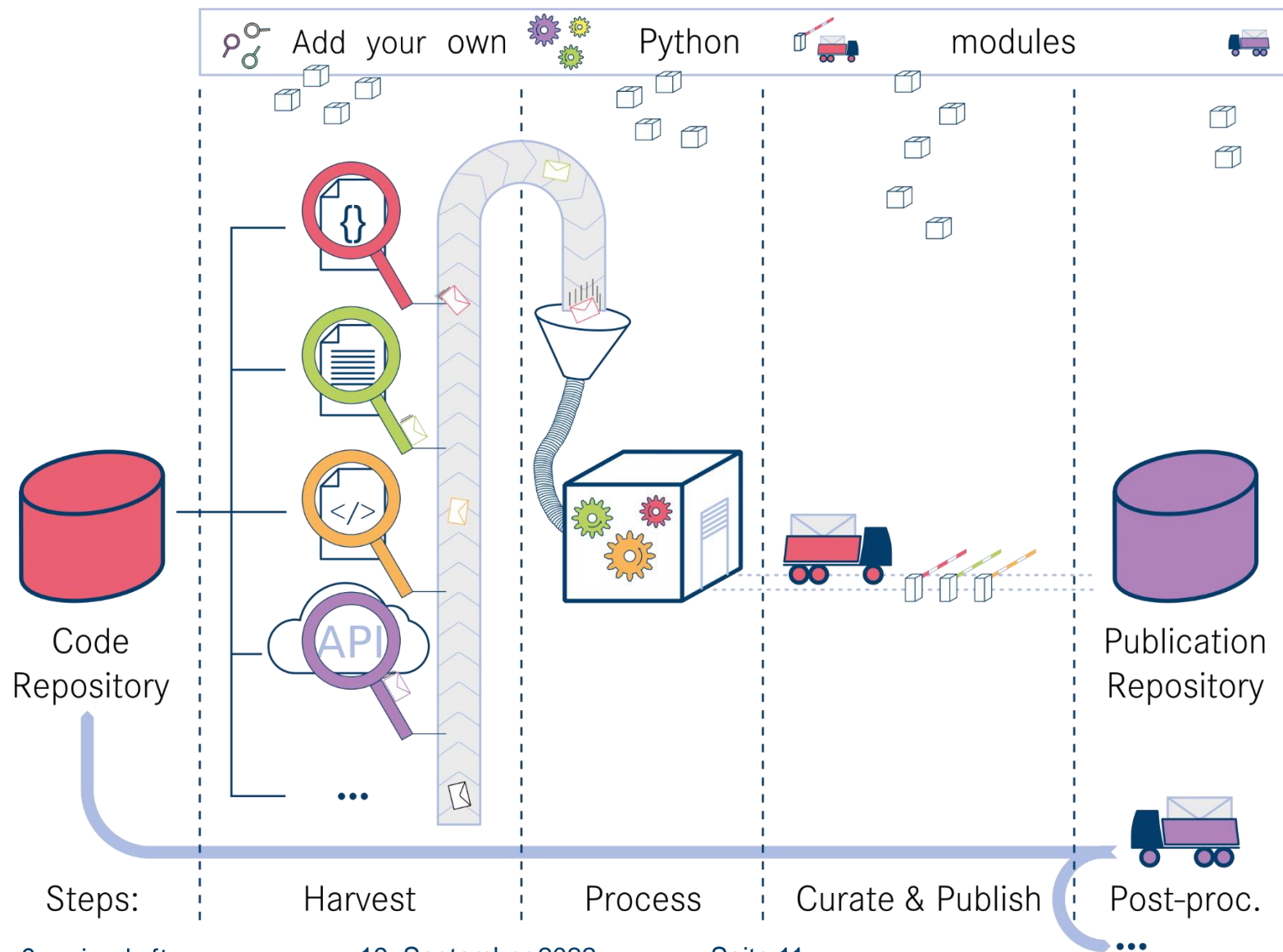


Where we are:

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

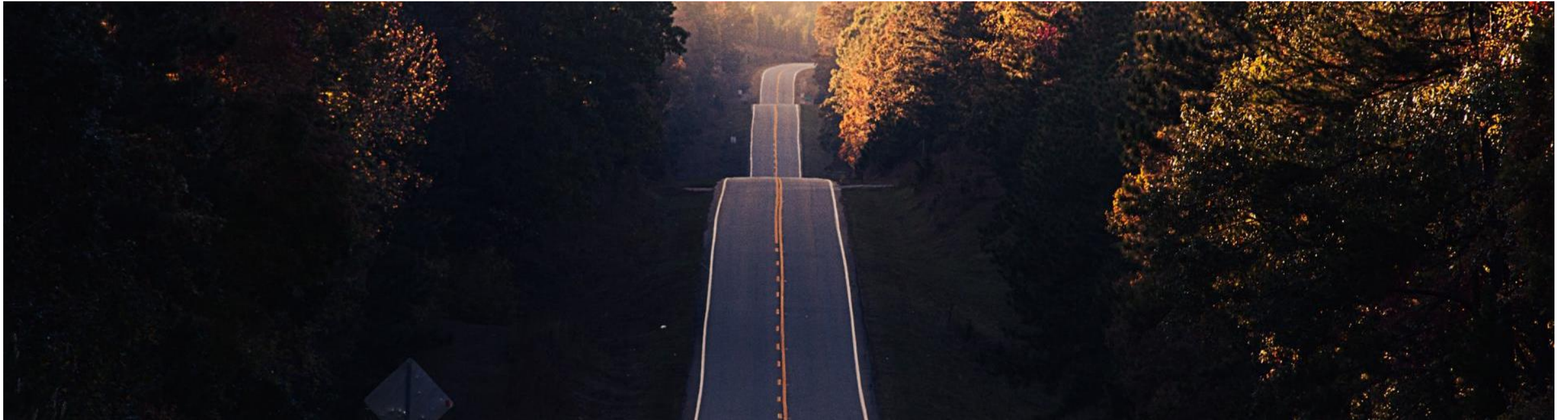
HERMES: CONCEPT II

Follow us on 
[hermes-hmc/workflow](https://github.com/hermes-hmc/workflow)



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



THANK YOU

TEAM@SOFTWARE-METADATA.PUB

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

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)