

# PROJECT HERMES

Easing the path to FAIR software publications



09.12.2022 | OLIVER BERTUCH<sup>1</sup>, STEPHAN DRUSKAT<sup>2</sup>, OLIVER KNODEL<sup>3</sup>, GUIDO JUCKELAND<sup>3</sup>,  
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DOI [10.5281/zenodo.7387926](https://doi.org/10.5281/zenodo.7387926)



... AND  
SOFTWARE!

# SOFTWARE PUBLICATION

# SOFTWARE PUBLICATION

## Software publication

enables

Sustainability

enables

Reproducibility

enables

Academic credit

enables



# SOFTWARE PUBLICATION: STATE OF THE ART

```

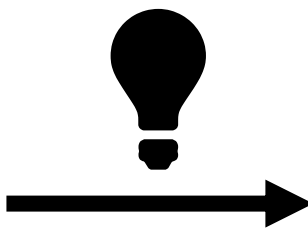
model = getattr(spectra, spectrum_dict["type"])

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 NameError(
            "Normalisation type not supported"
        )

    @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 1.2 kB
      - test.yml 403 Bytes
    - gignore 19.5 kB
    - pylintrc 1.9 kB
    - zenodo.json 1.5 kB
    - LICENSE 322 Bytes
    - MANIFEST.in 2.4 kB
    - README.md 202 Bytes
    - agnpy
      - \_\_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		
md5:87c5a702438f2aa3d6106d1cafb0204			

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... Daililar, Y. et al. 2021 ADS ARXIV
- ADS: 2021arXiv211112926M ADS ARXIV

768 views See more details... 157 downloads

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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>

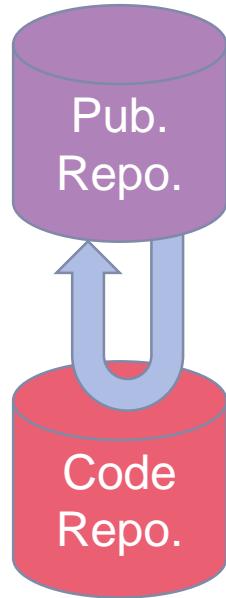
Communities: ESCAPE 2020

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

Versions

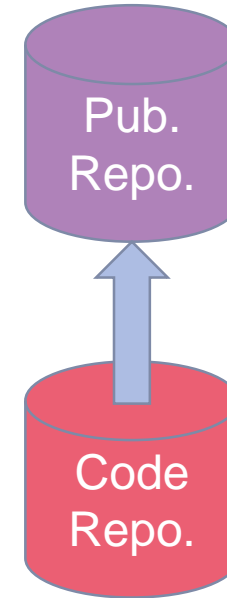
Version	Date
Version 0.1.8 10.5281/zenodo.5932850	Jan 31, 2022
Version 0.1.7 10.5281/zenodo.5927787	Jan 31, 2022

# 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

# RESEARCH SOFTWARE READINESS

## Publishing platforms:

- InvenioRDM based (i.e. Zenodo)
- Dataverse
- MyCoRe
- DSpace
- ...

## Criteria:

- Software metadata support
- Use existing standards (CodeMeta, CFF, OntoSoft, ...)
- Intake from harvesting / API / OAI-ORE / ...
- Make searchable & findable
- Visualize in UI
- Register as software with PID providers
- Export as CodeMeta & others for download
- Export as XML-RDF for harvesting via OAI-PMH
- Export as JSON-LD for SEO
- Machine-readable deposit metadata requirements
- Concept PID & Version PID (FAIR4RS F1)
- Reserve PID for draft version
- Software licenses support (CC ain't sufficient)
- Distinguishable data and software deposits



# 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](https://software-metadata.pub)

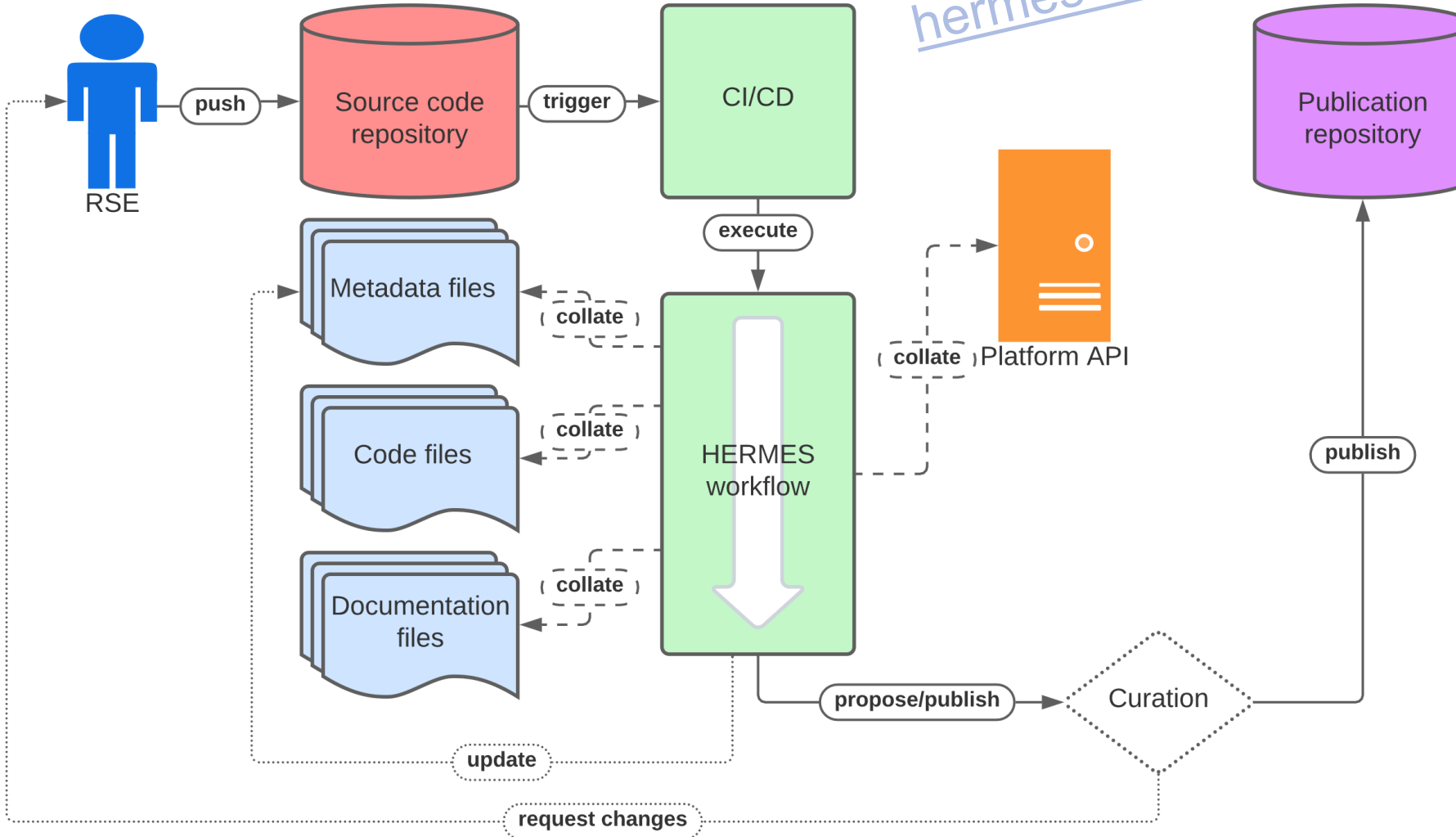


# HERMES: OUTPUTS (FOR THIS ITERATION)

- **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)

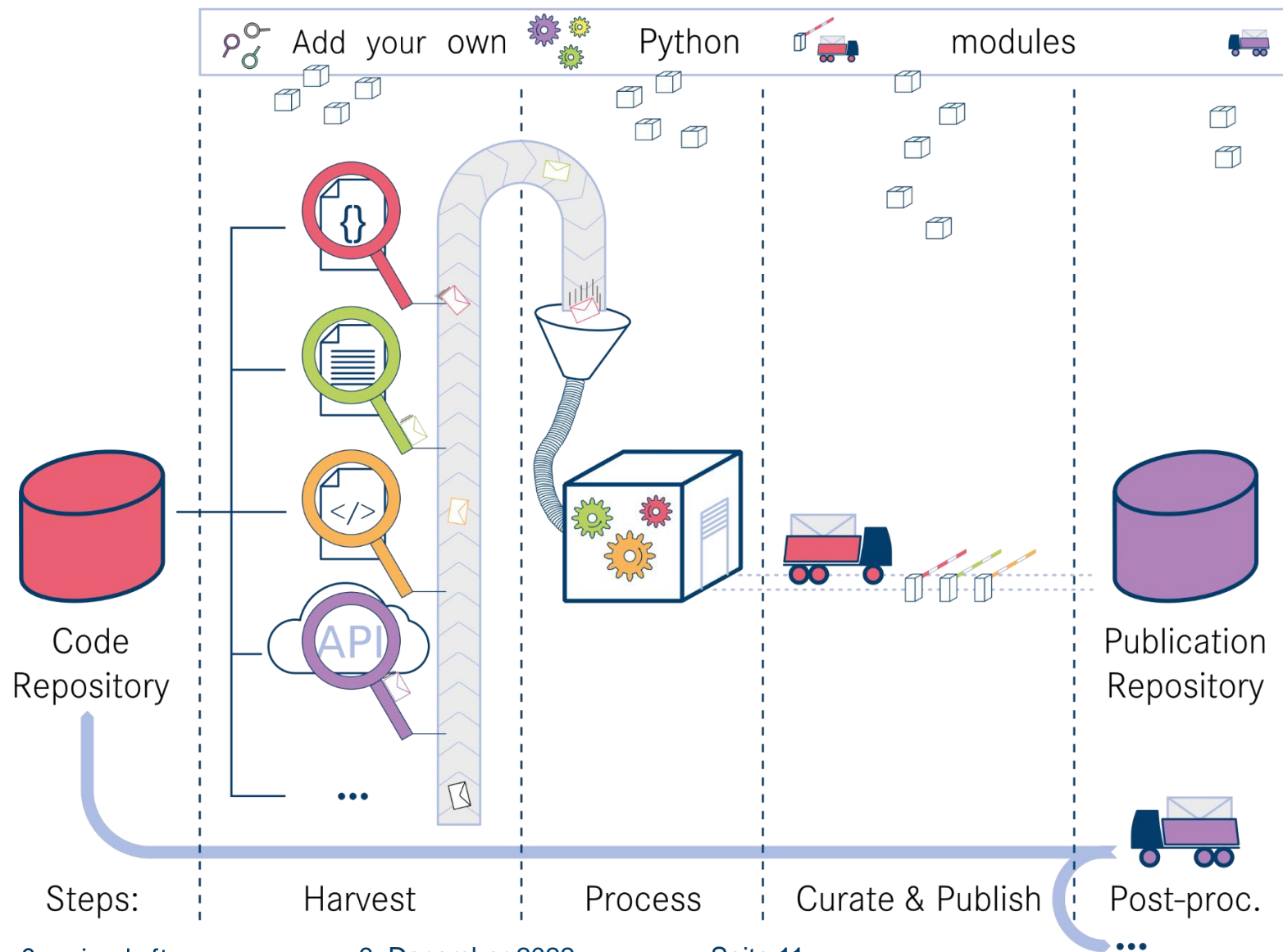


## Where we are:

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

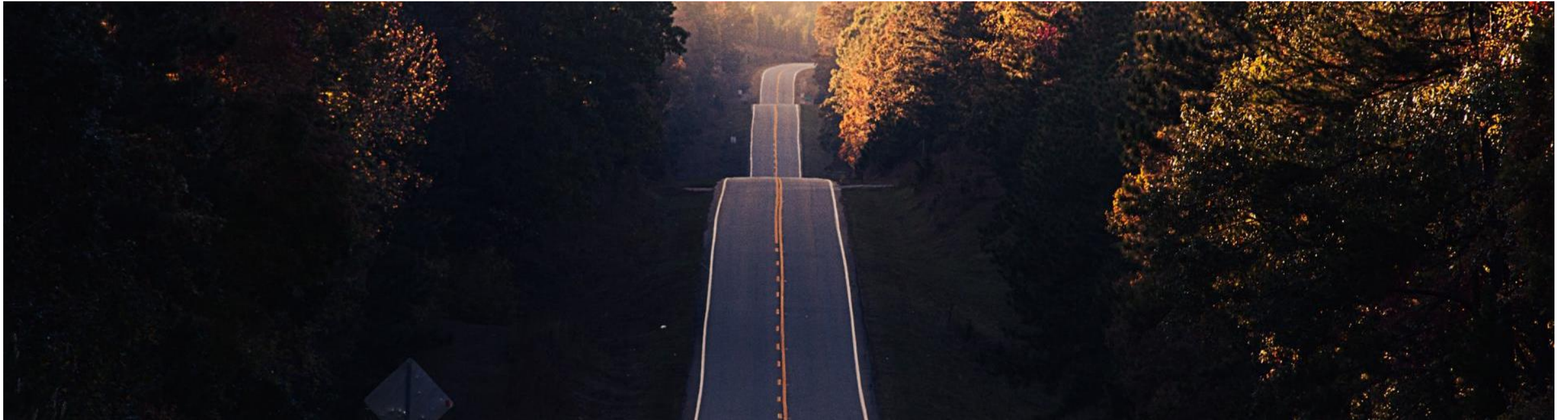
# HERMES: CONCEPT II

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



# HERMES: OUTLOOK

- **First project iteration ends 2022-06-30:**
  - Automated research software publication with rich metadata
- **Potential future work:**
  - “Research Software Readiness” of targets
  - New target repositories:
    - SURESOFT (TU Braunschweig)
    - Helmholtz research software directory?
    - NFDI publication repositories?
  - New metadata types via extended metadata mining
  - Curation: integrations, workflow, metrics, QA, ...?
  - Support for research software KPIs
  - New use cases (e. g. Carpentries, mixed deposits, ...)



# THANK YOU

[TEAM@SOFTWARE-METADATA.PUB](mailto: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)