

Helmholtz Quality Indicators for Software– & Data Products

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Program-Oriented Funding – Quality Indicator

Mandate of the Helmholtz Members Assembly (2022):

- Development of a multidimensional quality indicator for data products

Goals:

- Broadening / Improvement of the evaluation of science within Helmholtz
- Improving the visibility and recognition of diverse research outputs beyond text publications.
- Improving the quality and reusability of published research data
- Promotion of Open Science Practices

Expansion of the mandate to include the aspect of research software



Open Research Data

All Centers will establish detailed procedures for ensuring research data is publicly available, accessible and will regularly update and if necessary adapt these procedures.

By 2025, a basic indicator for the presentation of citable research data publications will be established and will be used for the evaluation of the PoF.

By 2028, a Helmholtz quality indicator for research data publications will be developed and established, which will be employed within the framework of the PoF and will include the aforementioned basic indicator.

Open Research Software

All Centers will aim to establish detailed research software management procedures in publicly available policies by 2025.

A specific indicator for the presentation of citable research software publications will be established in 2025 and will be used within the framework of the PoF together with research data publications.

By 2028, a Helmholtz quality indicator for research software publications will be developed and established, which will be employed within the framework of the PoF and will include the aforementioned basic indicator.

Task Group

Helmholtz Quality Indicators for Data and Software Products

- The [Task Group Helmholtz Quality Indicators for Data and Software Products](#) of the Working Group Open Science of the Helmholtz Association is dedicated to the development of Helmholtz Quality Indicators for Data and Software Products.
- Duration of TG: From March 2022 onwards;
- Inclusive approach: Representatives of all Helmholtz Centers
- Work in 3 groups: 1. Whole group ; 2. Sub-group research data ; 3. Sub-group research software
- Since reporting year 2023 (pub=2022): basic indicator for the presentation of citable research data publications was established as an incentive within the framework of the PoF
- Development of “Quality indicator”



Consensus and approach: multidimensional indicators

Make the indicator valuable for all involved

Cover all aspects of research data and software (tiers, types, research field)

Focus on the quality of the processes

Rely indicator on generic well-established concepts

Align the indicator with intended objectives not technical conditions

Iterative and inclusive process with all people involved

1. Definition of suitable dimensions for assessing the quality of RD- & RSW-publications
2. Collection of specific attributes for each dimension
3. Application of a generic maturity model to the attributes to be able to assign numerical values for maturity levels in each attribute
4. Determining the maturity level for each dimension, based on weighted average values of the dimension's attributes
5. Summarized quality assessment

Define quality dimensions and attributes

Adapting/Modifying FAIR-Principles



Wilkinson, M. et al. (2016).
<https://doi.org/10.1038/sdata.2016.18>



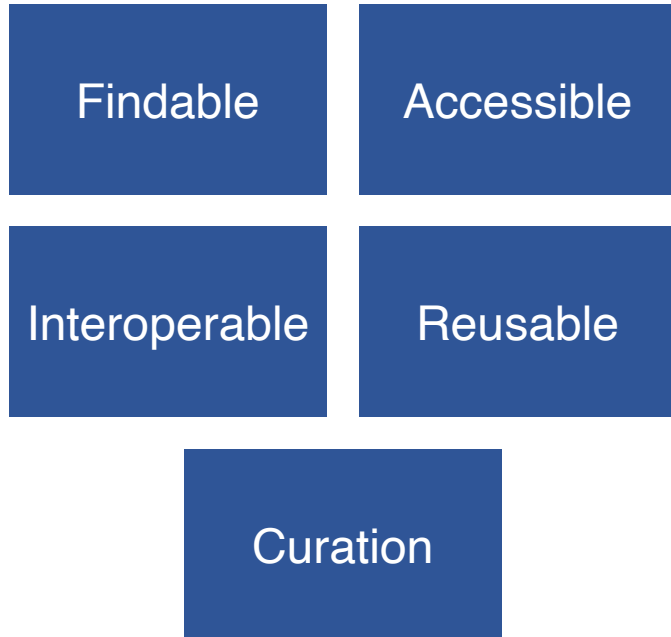
RDA FAIR Data Maturity Model Working Group (2020).
<https://doi.org/10.15497/rda00050>



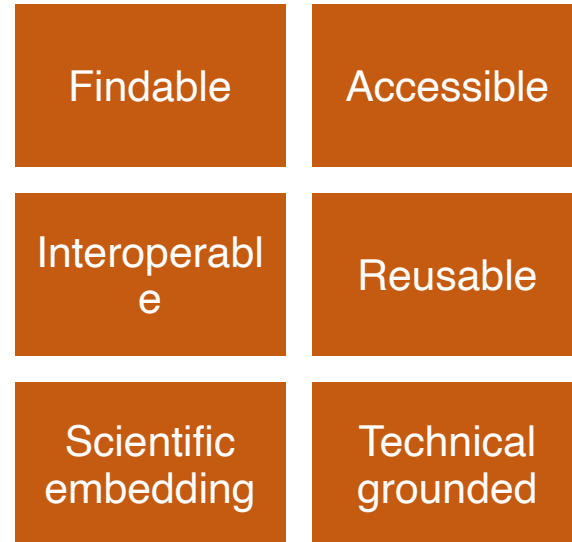
Chue Hong, N. P. et al. (2021). FAIR Principles for Research Software (FAIR4RS Principles). Research Data Alliance. <https://doi.org/10.15497/RDA00065>

Defined quality dimensions – based on FAIR/FAIR4RS

FAIR-C (Data)



FAIR-ST (Software)

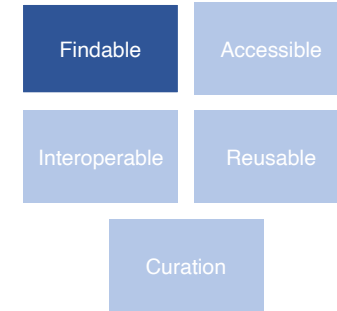


Defined attributes & how to measure them

Attributes = relevant aspects of quality in this one dimension

Example dimension „Findable“ (Software)

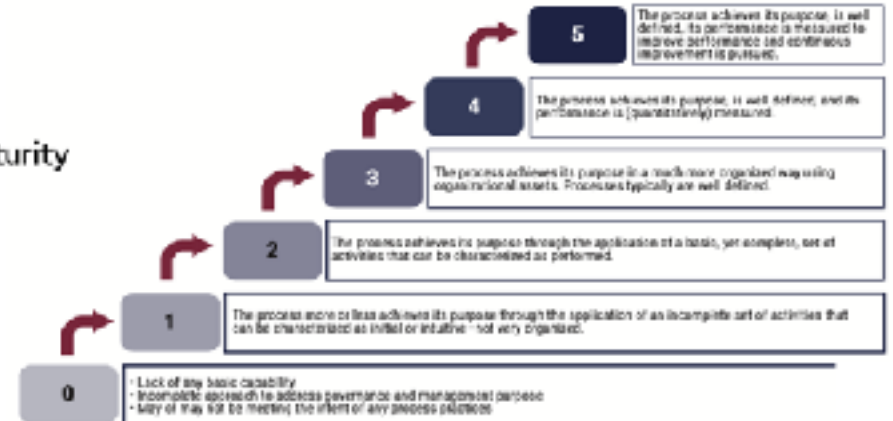
- Open Publication Repository
- Versioning
- Published with identifier
- Rich Metadata



Measuring attributes:

Using the COBIT maturity model

- generic international recognized framework to assess the maturity level of IT processes
- adapted and modified for indicator
- definition of maturity levels for each attribute



Maturity levels

Example data publication, dimension „Findable“

- **Maturity levels for attribute** „Open Publication Repository“

(0) There is no information available on where to find the software.

(1) The software is contained in an online repository.

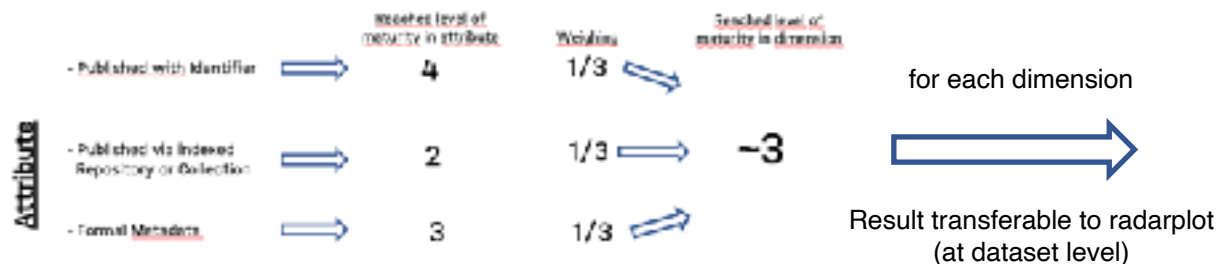
(2) Some kind of description is available giving further information on the software in this repository (e.g. readme file).

(3) A structured meta data description (e.g. following DataCite) given for software is in this repository.

(4) The repository is listed in some overarching meta-repository (e.g. Helmholtz Research Software Directory (RSD), re3data).

Aggregation

Aggregating per Dimension by weighted attributes, Example: dimension „Findable“



How to aggregate at Center-level?

- Definition of a „minimum polygon“ for data/sw publications (Red line, illustration exemplary)
- If data publication meets the minimum: count as „1“

Incentive to improve quality?

- The minimum polygon can be raised over time to incentivize the improvement of data publications

How (Specific to reserach data publications)

Paper and Pencil-exercise with actual software and data publications

- by groups from different research areas / centers
- Results/ insight:
 - the concept generally works
 - there are currently limited possibilities of automation
 - data publications within a single repository usually receive a similar results (Helmholtz/domain/insitutional)
- Conclusion for sub-group data:
 - evaluation of some attributes postponed; to be implemented later
 - first implementation step via looking at repository level: assumption from P&P
 - Automatisatation at dataset-level is adressed at later point to keep it feasible

A screenshot of a data table with a light orange background and a yellow header bar. The table contains multiple columns and rows of data.

A screenshot of a data table with a yellow background and a green vertical bar. The table contains multiple columns and rows of data.

A screenshot of a data table with a yellow background and a green vertical bar. The table contains multiple columns and rows of data.

The content of this page is subject to change without notice. The information provided here is for informational purposes only and does not constitute an offer or recommendation. The information is provided as is and is not guaranteed to be accurate, complete, or up to date. Please contact the source of the information for more details.

How (Specific for research software publications)

Check if research software publication qualifies

- Has author from the reporting center
- Qualifies as research software (in contrast to infrastructure software → can be counted as transfer)
- Max. one software release per year (as software is a living object with constant updates)

Evaluation of each individual publication

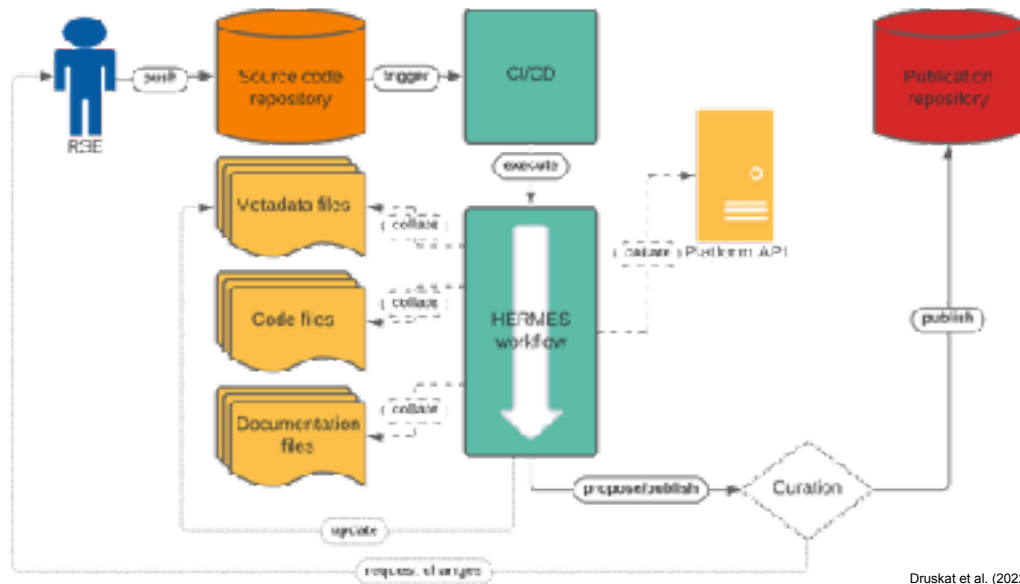
- Automated through tools
 - Either via the authors themselves by entering the software into the Helmholtz Research Software Directory (RSD)
 - Or via a center specific process that can use the provided tools for evaluation (published as open-source)
- Not all attributes and maturity can currently be covered by automated tools → skipped in evaluation until tools are available

HERMES: Helmholtz Rich Metadata Software Publication

(HMC project ZT-I-PF-3-006, 7/21-12/23, DLR + FZJ + HZDR)



- Automated software publication for all platform combinations
- Use existing metadata to enrich records/improve FAIRness
- Enable:
 - closed source publication,
 - curation & sign-off processes,
 - updating metadata records



Druskat et al. (2022)

■ software-metadata.pub



HERMES: Implementation

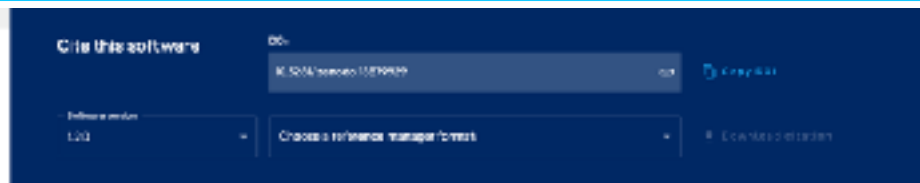


- Continuous integration workflow: on <event> run hermes as configured
- Tutorials for GitHub/GitLab: docs.software-metadata.pub



- hermes Python package (Meinel et al. 2024) + CI templates (GitHub, GitLab)
- Plugins via Python Extension Point mechanism for each step
- Details: Kernchen et al. (2024)

Helmholtz RSD as one place for all the metadata



What alpaka can do for you

The **alpaka** library is a header-only C++ abstraction library for accelerator developers.

It aims to provide performance portability across accelerators through the abstraction and hiding of the underlying levels of parallelism.

It is platform-agnostic and supports the execution of an application on multiple accelerators on the host CPU (x86, ARM, PPC-32 and PowerPC) and GPU accelerators from all major vendors (NVIDIA, AMD, and Intel).

A multitude of accelerator back-end variants using CUDA, HIP, SYCL, OpenMP-5.0, and others, and auto-serial execution is provided and available on some regarding the device.

Only one implementation of the user-handled required by recompiling the main function object with the special interface.

There is no need to write special CUDA, HIP, SYCL, OpenMP or custom threading code.

Accelerator back-end choice for individual system level for the compilation as a choice.

The device which accelerator back-end should be used for which hardware is made at runtime.

With its robust development and testing standards, **alpaka** ensures a software-ready solution for both industry and research applications, making it a versatile tool for high-performance computing.

Related projects

HiConGPU

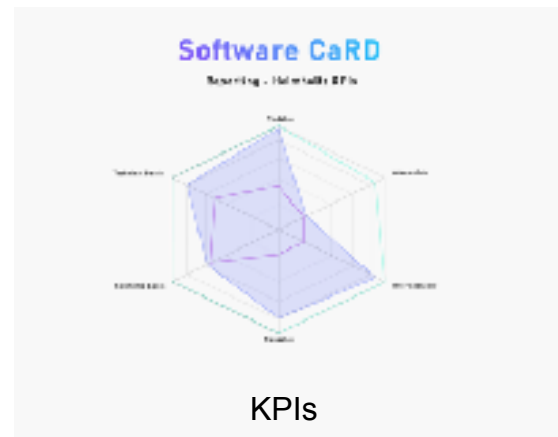
HiConGPU is an extremely scalable and platform-parallel application for particle-pair simulations. While we really care if its daily use in physics and astrophysics, it has also been used for other scientific applications of machine learning in various conditions.

Current work: hermes 1.0.0, Software CaRD



- hermes 1.0.0
- Software Curation and Reporting Dashboard (Software CaRD)
 - Input: Consistent knowledge graph produced by HERMES
 - Compliance checks against configurable policies (KPIs, curation)
 - HMC project (2023 cohort; DLR + HZDR + GFZ + FZJ)

```
graph TD
    subgraph "Software CaRD"
        direction TB
        A[Input: Consistent knowledge graph produced by HERMES] --> B[Compliance checks against configurable policies (KPIs, curation)]
        B --> C[HMC project (2023 cohort; DLR + HZDR + GFZ + FZJ)]
    end
```



Software CaRD Curation Dashboard

| NAME | EMAIL | ORCID | STATUS | LAST UPDATE |
|------------------------|----------------------|---------------------|--------|---------------------|
| John F. Jones | john.f.jones@dlr.de | 0000-0001-2345-6789 | Active | 2023-10-27 10:30:00 |
| Jane Doe | jane.doe@dlr.de | 0000-0002-3456-7890 | Active | 2023-10-27 10:30:00 |
| Michael Smith | michael.smith@dlr.de | 0000-0003-4567-8901 | Active | 2023-10-27 10:30:00 |
| E-Mail address [email] | michael.smith@dlr.de | 0000-0004-5678-9012 | Active | 2023-10-27 10:30:00 |
| Nickname [nickname] | michael.smith@dlr.de | 0000-0005-6789-0123 | Active | 2023-10-27 10:30:00 |

Curation

What to report?

Research data
publications

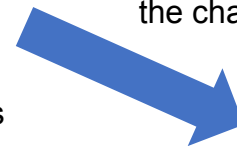
All research data publications with authors from your center published in the reporting year



Published in a listed and evaluated data repository



Repository fulfills min. criteria



A = Sum(all research data publications fulfilling the chain)

Research software
publications

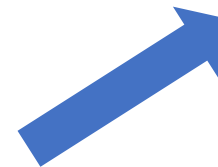
All research software publications with authors from your center published in the reporting year (max. 1 release)



Evaluated by tools or center process using the published criteria



Software publication fulfills min. criteria



B = Sum(all research software publications fulfilling the chain)

Indicator =
(A ; B)

Status quo and next steps for implementation 1/2

Assembly of members

- pre-approval of concept by directors working group in 7-8/2024
- adoption by assembly of members in 9/2024
 - positive reception of concept
 - praise for scientific approach

Proposed time horizon of the TG:

- introduction at the beginning of POF V for reporting year 2028 (data collection Q1/2029)
- reporting years (publication year) 2025 - 2027 test introduction (first test collection Q1/2026 = publication year 2025); [→ last use of basic indicator for reporting year 2024]

Work level TG

- optimize criteria catalogs by the end of 2024
- clarification overarching questions (versions/granularity, „authorship“, etc.)
- Definition of minimal-polygon
- prepare test introduction

Sub-group
meetings every two
weeks since
September 2024

Status quo and next steps for implementation 2/2

Initial training and feedback opportunities

- TG develops a handout for the application of the Indicator (Early Jan '25)
- virtual Q&A possibility for the level of „controllers“ (End of Jan '25; date will be announced asap)
- hands-on software for operational level (Mid Feb '25 @Research Software Forum)
- hands-on data for operational level (Apr/May '25 Workshop format, tba)

Work level TG 2025

- conceptualizing workflow for repository assessment (data)
- collecting information on repositories used at Helmholtz (data)
- identifying tools for automation and integrate them to a „toolbox“ (software)
- set-up of a centralized feedback possibility (both)

Goal: Mid 2025, to best prepare Centers in 2nd half 2025

The TG will accompany the test phase and will continuously incorporate lessons learned and collect best/good -practices to have established processes by start of POF V

Keep in touch



open-science@helmholtz.de



<https://os.helmholtz.de>



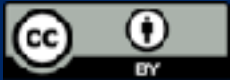
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