

Using an ensemble of FAIR assessment approaches to inform the design of future FAIRness testing: a case study evaluating World Data Center for Climate (WDCC)-preserved (meta)data

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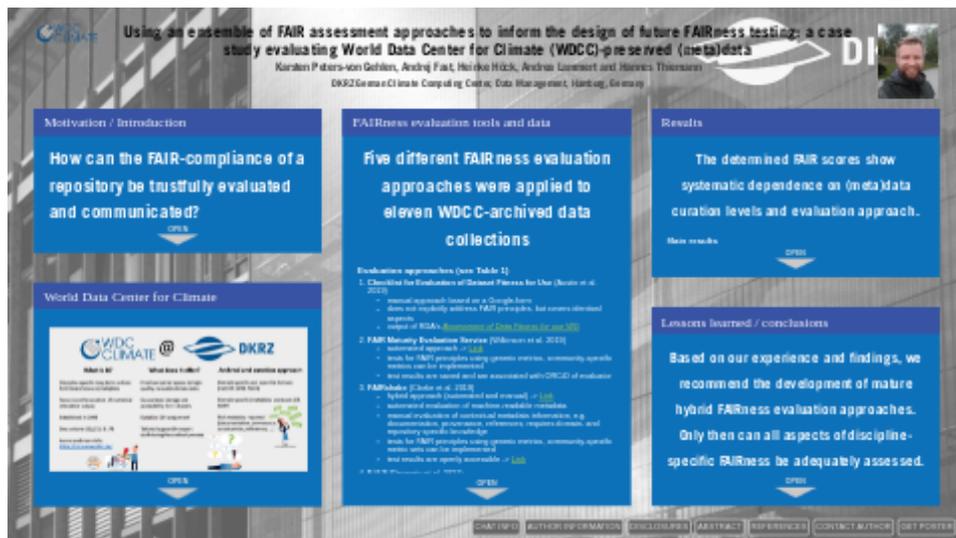
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Abstract

From a research data repositories' perspective, offering data management services in-line with the FAIR principles is becoming more and more of a selling point to compete on the market. In order to do so, the services offered must be evaluated and credited following transparent and credible procedures. Several FAIRness evaluation methods are openly available for being applied to archived (meta)data. However, there exists no standardized and globally accepted FAIRness testing procedure to date. Here, we apply an ensemble of 5 FAIRness evaluation approaches to selected datasets archived in the WDCC. The selection represents the majority of WDCC-archived datasets (by volume) and reflects the entire spectrum of data curation levels. Two tests are purely automatic, two are purely manual and one test applies a hybrid method (manual and automatic combined) for evaluation. The results of our evaluation show a mean FAIR score of 0.67 of 1. Manual approaches show higher scores than automated ones. The hybrid approach shows the highest score. Computed statistics show agreement between the tests at the data collection level. None of the five evaluation approaches is fully fit-for-purpose to evaluate (discipline-specific) FAIRness, but all have their merit. Manual testing captures domain- and repository-specific aspects of FAIR. Machine-actionability of archived (meta)data is judged by the evaluator. Automatic approaches evaluate the machine-actionable features of archived (meta)data. These have to be accessible by an automated agent and comply with globally established standards. An evaluation of contextual metadata (essential for reusability) is not possible. Correspondingly, the hybrid method combines the advantages and eliminates the deficiencies of manual and automatic evaluation. We recommend that future operational FAIRness evaluation be based on a mature hybrid approach. The automatic part of the evaluation would retrieve and evaluate as much machine-actionable discipline specific (meta)data content as possible and be then complemented by a manual evaluation focusing on the contextual aspects of FAIR. Design and adoption of the discipline-specific aspects will have to be conducted in concerted community efforts. We illustrate a possible structure of this process with an example from climate research.

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PRESENTED AT:



MOTIVATION / INTRODUCTION

How can the FAIR-compliance of a repository be trustfully evaluated and communicated?

Why is this important?

- scientists are by now often required to make their research data available to the community in-line with the FAIR data principles
- IT-infrastructure, i.e. a repository, must be in place to satisfy F, A and parts of R
- suitable repositories must be known to the scientists
- BUT: no commonly accepted method to assess the FAIR-compliance of repositories exists to date

What would be nice to have?

From the repositories' perspective:

- standardized approach to (discipline-specific) FAIRness evaluation minimizing the effect of evaluation biases
- agreed upon scoring system to communicate FAIR compliance

From the scientists' perspective:

- easy-to-access FAIRness scores by repository
- clearly communicated lists of available repositories complying with FAIR data principles

How can FAIRness be evaluated (end of 2021)?

- a multitude of different tools is available
 - manual questionnaires
 - automated tests accessing the online resources
 - hybrid approaches (automated and manual)
- recommendations for FAIR metrics/criteria to assess in an evaluation have been collected in a community activity (RDA, Bahim et al. 2020)
 - basis for self-designed FAIRness evaluation

What is the problem then?

- available evaluation tools cover the FAIR dimensions (F, A, I, R are considered "dimensions" here) in different depth
- FAIR dimensions are not evaluated consistently between approaches
- no common approach to calculate FAIR scores is defined
- manual vs automated approaches yield different results by nature of their design
- FAIR scores of repositories cannot be compared, unless the same evaluation approach was used
- **repository providers and scientists are faced with the dilemma of inconsistent and possibly subjective FAIRness scores making it impossible to**
 - **communicate repository FAIRness (repository's perspective)**
 - **choose an appropriate repository for making (meta)data available (scientists' perspective)**

What is the aim of this study?

We aim to contribute to the development of future operational FAIRness evaluation approaches by assessing the FAIRness of (meta)data preserved in the WDCC (World Data Center for Climate, see below for more information) using multiple evaluation tools.

In doing so, we

- get an impression of the user-friendliness of the different evaluation approaches

- get an impression of the comparability of the different evaluation tools
- learn about benefits and shortcomings of different evaluation approaches
- provide recommendations for the design of future FAIRness evaluation approaches
- provide a sound estimate of the FAIRness of WDC-archived (meta)data

WORLD DATA CENTER FOR CLIMATE



What is it?	What does it offer?	Archival and curation approach
Discipline-specific long-term archive for Climate Science (meta)data	Free low-barrier access to high-quality, reusable climate data	Domain specific and open file formats (netCDF, GPB, ASCII)

For climate science (meta)data	quality, reusable climate data	(netCDF, GRIB, ASCII)
Focus is on the curation of numerical simulation output	Guaranteed storage and accessibility for >10 years	Domain specific (meta)data standards (CF, CMIP)
Established in 2003	DataCite DOI assignment	Rich metadata required (documentation, provenance, uncertainties, references, ...)
Data volume (12/21): 3.1PB	Tailored support by expert staff during the archival process	
Access and more info: https://cera-www.dkrz.de/		

See <https://cera-www.dkrz.de/> (<https://cera-www.dkrz.de/>) for more information.

FAIRNESS EVALUATION TOOLS AND DATA

Five different FAIRness evaluation approaches were applied to eleven WDC-archived data collections

Evaluation approaches (see Table 1)

1. **Checklist for Evaluation of Dataset Fitness for Use** (Austin et al. 2019)
 - o manual approach based on a Google-form
 - o does not explicitly address FAIR principles, but covers identical aspects
 - o output of RDA's *Assessment of Data Fitness for use WG* (<https://rd-alliance.org/node/54458/outputs>)

2. **FAIR Maturity Evaluation Service** (Wilkinson et al. 2019)
 - automated approach -> Link (<https://fairsharing.github.io/FAIR-Evaluator-FrontEnd/#!//#%2F!>)
 - tests for FAIR principles using generic metrics, community-specific metrics can be implemented
 - test results are saved and are associated with ORCID of evaluator
3. **FAIRshake** (Clarke et al. 2019)
 - hybrid approach (automated and manual) -> Link (<https://fairshake.cloud>)
 - automated evaluation of machine-readable metadata
 - manual evaluation of contextual metadata information, e.g. documentation, provenance, references; requires domain- and repository specific knowledge
 - tests for FAIR principles using generic metrics, community-specific metric sets can be implemented
 - test results are openly accessible -> Link (<https://fairshake.cloud/project/>)
4. **F-UJI** (Devaraju et al. 2021)
 - automated approach, available as installable package or web-based application -> Link (<https://www.f-uji.net>)
 - tests for FAIR principles using generic metrics, while also applying domain-specific criteria by sourcing external resources
 - results are displayed in a dashboard-like manner for the web-based application; saving online is not possible
5. **Self Assessment**
 - manual approach based on the recommended FAIR metrics published in Bahim et al. (2020)
 - tests for FAIR principles using generic metrics; completing the evaluation requires expert domain- and repository-specific knowledge

Tool	Acronym	method	Covered FAIR dimensions	Reference
Checklist for Evaluation of Dataset Fitness for Use	CFU	manual	n/a	Austin et al. (2019)
FAIR Maturity Evaluation Service	FMES	automated	F: 8, A: 5, I: 7, R: 2	Wilkinson et al. (2019)
FAIRshake	n/a	hybrid	F: 3, A: 1, I: 0, R: 5	Clarke et al. (2019)
F-UJI	n/a	automated	F: 7, A: 3, I: 4, R: 10	Devaraju et al. (2021)
Self Assessment	n/a	manual	F: 13, A: 12, I: 10, R: 10	Bahim et al. (2020)

Table 1: Summary of the five FAIRness evaluation tools used in this study. The hybrid method of FAIRshake combines automated and manual evaluation. The covered FAIR ((F)indable, (A)ccessible, (I)nteroperable, (R)eusable) dimensions refer to the number of metrics the tool tests, e.g. FMES checks for Findability using 8 different tests.

Evaluated data collections (see Table 2)

- A subset of WDCC-archived (meta)data representative for the majority of WDCC data holdings (by volume, see Table 2) was chosen for evaluation.
- The chosen data collections feature different levels of data curation and therefore also provide an overview of the breadth of WDCC-archived assets
- The chosen data are comprised of CMIP model simulation output, observational datasets, institutional modelling efforts and campaign data
- As data collections are seen representative of entire projects, the evaluated (meta)data represent 65% of the WDCC holdings by volume

Project acronym	Data summary	Project volume [TB]	DOI assigned	Creation date	Comments
IPCC-AR5_CMIP5	Coupled Climate Model Output, prepared following CMIP5 guidelines and basis of the IPCC 5th Assessment Report (2 AICs evaluated)	1655	yes and no	2012-05-31 and 2011-10-10	
CliSAP	Observational data products from satellite remote sensing (2 AICs evaluated)	163	yes and no	2015-09-15 and 2009-11-12	one collection with no data access
WASCAL	Dynamically downscaled climate data for West Africa	73	yes	2017-02-23	
CMIP6_RCM_forcing_MPI-ESM1-2	Coupled Climate Model output prepared as boundary conditions for regional climate models, prepared following CMIP6 experiment guidelines	51	yes	2020-02-27	
MILLENNIUM_COSMOS	Coupled Climate Model of ensemble simulations covering the last millenium (800-2000AD)	47	no	2009-05-12	
IPCC_TAR_ECHAM4/OPYC	Coupled Climate Model Output, prepared to support the IPCCs 3rd Assessment Report	2.6	yes	2003-01-26	Experiment and dataset with DOI; First ever DOI assigned to data (Stendel et al., 2004)
Storm_Tide_1906_German_Bight	Numerical simulation of the 1906 storm tide in the German Bight	0.3	yes	2020-10-27	

COPS	Observational data obtained from radar remote sensing during the COPS (Convective and Orographically-Induced Precipitation Study) campaign	0.2	yes	2008-01-28
HDCP2-OBS	Observations collected during the HDCP ² (High Definition Clouds and Precipitation for Climate Prediction) project	0.06	yes	2018-09-18
OceanRAIN	In-situ, along-track ship-board observations of routinely measured atmospheric and oceanic state parameters over global oceans	0.01	yes	2017-12-13 7
CARIBIC	Observations of atmospheric parameters obtained from commercial aircraft equipped with an instrumentation container	7.7E-5	no	2002-04-27

Table 2: WDCC projects selected for evaluation. The project acronyms can be directly used to search and find the evaluated projects using the WDCC GUI. The project volume in TB (third column) refers to the total volume of the entire project named in the first column. A full listing with more comprehensive information on the evaluated WDCC-entries is provided in the spreadsheets underlying this study (cf Supplement).

RESULTS

The determined FAIR scores show systematic dependence on (meta)data curation levels and evaluation approach.

Main results

- manual or hybrid approaches yield higher FAIR scores compared to automated approaches (Table 3)
- high (meta)data curation levels yield higher FAIR scores (and vice versa) across all applied evaluation tools (Table 3)
- agreement between test approaches is fair, with a few exceptions showing good agreement (Table 4)

Availability of results

- all results are published in WDCC and openly available
 - csv tables of evaluation results and statistics: Link (https://doi.org/10.35095/WDCC/Results_from_FAIRness_eval)
 - PDF printouts of F-UJI test results: Link (https://doi.org/10.35095/WDCC/F-UJI_results_WDCC)

Comparability of results

- we applied equal weighting to every tested metric in each evaluation approach and normalized the results
- automated approaches provided binary yes/no results per test only, resulting in a score of either 0 (no) or 1 (yes) per metric
- manual approaches also allowed for nuanced answers in the range of 0..1 per metric

Calculated statistics

- apart from the mean FAIR score per project averaged over all five tests (third column from right in Table 3) we also computed the absolute and relative standard deviation per project (rightmost two columns of Table 3). Especially the relative standard deviation provides an impression of agreement between the tests on a project level.
- we analyse the general agreement between the test approaches through cross-correlations (Table 4)

- we analyse the general agreement between the test approaches through cross-correlations (Table 7)

Project acronym	Self Assessment	CFU	FMES	F-UJI	FAIRshake	\emptyset per project	σ per project	$\frac{\sigma}{\emptyset}$ per project
IPCC-AR5_CMIP5	0.84	0.72	0.44	0.58	0.95	0.71	0.20	0.29
IPCC-AR5_CMIP5, no DOI	0.65	0.67	0.44	0.54	0.93	0.65	0.19	0.29
CliSAP	0.86	0.78	0.48	0.58	0.97	0.73	0.20	0.28
CliSAP, no data accessible	0.27	0.30	0.43	0.52	0.64	0.43	0.15	0.36
WASCAL	0.90	0.80	0.50	0.58	0.91	0.74	0.18	0.25
CMIP6_RCM_forcing_MPI-ESM1-2	0.86	0.85	0.57	0.62	0.92	0.76	0.16	0.21
MILLENNIUM_COSMOS	0.63	0.53	0.45	0.51	0.82	0.59	0.14	0.24
IPCC_TAR_ECHAM4/OPYC	0.82	0.63	0.50	0.64	0.89	0.70	0.16	0.23
Storm_Tide_1906_German_Bight	0.90	0.68	0.55	0.62	0.83	0.71	0.15	0.21
COPS	0.86	0.47	0.53	0.55	0.87	0.66	0.19	0.29
HDCCP2-OBS	0.90	0.48	0.53	0.59	0.86	0.67	0.19	0.29
OceanRAIN	0.90	0.75	0.57	0.60	0.97	0.76	0.18	0.23
CARIBIC	0.62	0.70	0.50	0.54	0.82	0.64	0.13	0.20
\emptyset (WDCC)	0.77	0.64	0.50	0.58	0.88	0.67	0.15	0.22

Table 3: Results of FAIR assessments of WDCC data holding using the ensemble of FAIRness evaluation tools detailed in Section 2.1. The scores per test are calculated as unweighted mean over all tested FAIR maturity indicators. The mean (\emptyset), standard deviation (σ) and relative standard deviation ($\frac{\sigma}{\emptyset}$) on a project basis (three rightmost columns) are calculated across the scores of the five FAIR assessment tools. The mean value representative for the WDCC (\emptyset (WDCC), last row) is calculated for all values in the respective column of the table. See main text for more details. Results at finer granularity are provided in the supporting data (Peters-von Gehlen & Hoeck, 2021)

	Self Assessment	CFU	FMES	F-UJI	FAIRshake
Self Assessment	n/a	0.61	0.65	0.73	0.79
CFU		n/a	0.36	0.50	0.78
FMES			n/a	0.65	0.30
F-UJI				n/a	0.49
FAIRshake					n/a

Table 4: Cross-correlations between the scores per project obtained with the five FAIRness evaluation tools (Table 3).

LESSONS LEARNED / CONCLUSIONS

Based on our experience and findings, we recommend the development of mature hybrid FAIRness evaluation approaches. Only then can all aspects of discipline-specific FAIRness be adequately assessed.

This is because:

- automated approaches have limitations assessing the **contextual reusability** of data
- manual approaches have - naturally - **limitations assessing the machine actionability** of archived research data
- hybrid approaches provide the best of both worlds

Developing mature hybrid approaches will require coupling a technically capable automated approach - as already provided by e.g. F-UJI - together with manual forms which are efficient to complete. The applied metrics will have to be developed through community-driven processes in order to ensure domain-specific aspects are properly taken into account.



DISCLOSURES

This content is currently under review for publication with Data Science Journal.

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Work Area

- Communication, mediation and integration of DKRZ research data management services for the Earth System Science Community
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- working at DKRZ since April 2018

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Meteorology and climate science:

- Diploma of Meteorology (equivalent to MSc, University of Hamburg), 2008
- PhD in Meteorology (University of Hamburg, Max Planck Institute for Meteorology), 2011
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ABSTRACT

From a research data repositories' perspective, offering data management services in-line with the FAIR principles is becoming more and more of a selling point to compete on the market. In order to do so, the services offered must be evaluated and credited following transparent and credible procedures. Several FAIRness evaluation methods are openly available for being applied to archived (meta)data. However, there exists no standardized and globally accepted FAIRness testing procedure to date.

Here, we apply an ensemble of 5 FAIRness evaluation approaches to selected datasets archived in the WDCC. The selection represents the majority of WDCC-archived datasets (by volume) and reflects the entire spectrum of data curation levels. Two tests are purely automatic, two are purely manual and one test applies a hybrid method (manual and automatic combined) for evaluation.

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None of the five evaluation approaches is fully fit-for-purpose to evaluate (discipline-specific) FAIRness, but all have their merit. Manual testing captures domain- and repository-specific aspects of FAIR. Machine-actionability of archived (meta)data is judged by the evaluator. Automatic approaches evaluate the machine-actionable features of archived (meta)data. These have to be accessible by an automated agent and comply with globally established standards. An evaluation of contextual metadata (essential for reusability) is not possible. Correspondingly, the hybrid method combines the advantages and eliminates the deficiencies of manual and automatic evaluation.

We recommend that future operational FAIRness evaluation be based on a mature hybrid approach. The automatic part of the evaluation would retrieve and evaluate as much machine-actionable discipline specific (meta)data content as possible and be then complemented by a manual evaluation focusing on the contextual aspects of FAIR. Design and adoption of the discipline-specific aspects will have to be conducted in concerted community efforts. We illustrate a possible structure of this process with an example from climate research.

REFERENCES

- Austin, C., Cousijn, H., Diepenbroek, M., Petters, J. and Soares E Silva, M., 2019, WDS/RDA Assessment of Data Fitness for Use WG Outputs and Recommendations, doi:10.15497/rda00034.
- Bahim, C., Casorr'an-Amilburu, C., Dekkers, M., Herczog, E., Loozen, N., Repanas, K., Russell, K. and Stall, S., 2020, The FAIR Data Maturity Model: An Approach to Harmonise FAIR Assessments, *Data Sci. J.*, 19, 41, doi:10.5334/dsj-2020-041.
- Clarke, D. J., Wang, L., Jones, A., Wojciechowicz, M. L., Torre, D., Jagodnik, K. M., Jenkins, S. L., McQuilton, P., Flamholz, Z., Silverstein, M. C., Schilder, B. M., Robasky, K., Castillo, C., Idaszak, R., Ahalt, S. C., Williams, J., Schurer, S., Cooper, D. J., de Miranda Azevedo, R., Klenk, J. A., Haendel, M. A., Nedzel, J., Avillach, P., Shimoyama, M. E., Harris, R. M., Gamble, M., Poten, R., Charbonneau, A. L., Larkin, J., Brown, C. T., Bonazzi, V. R., Dumontier, M. J., Sansone, S. A. and Ma'ayan, A., 2019, FAIRshake: Toolkit to Evaluate the FAIRness of Research Digital Resources, *Cell systems*, 9, 417–421, doi:10.1016/j.cels.2019.09.011.
- Devaraju, A., Mokrane, M., Cepinskas, L., Huber, R., Herterich, P., de Vries, J., Akerman, V., L'Hours, H., Davidson, J. and Diepenbroek, M., 2021, From Conceptualization to Implementation: FAIR Assessment of Research Data Objects, *Data Sci. J.*, 20, 4, doi: 10.5334/dsj-2021-004.
- Wilkinson, M. D., Dumontier, M., Sansone, S.-A., da Silva Santos, L. O. B., Prieto, M., Batista, D., McQuilton, P., Kuhn, T., Rocca-Serra, P., Crosas, M. and Schultes, E., 2019, Evaluating FAIR maturity through a scalable, automated, community-governed framework, *Sci. Data*, 6, 1–12, doi:https://doi.org/10.1038/s41597-019-0184-5.