

● Research Data Management for Data from HPC

Best-Practice and Applications

15/04/2024, 10:00-13:00



Speakers

Technical University of Munich (TUM)

Prof. Dr.-Ing. Christian Stemmer | Chair of Aerodynamics and Fluid Mechanics

Vasiliki Sdralia | Munich Data Science Institute | Chair of Aerodynamics and Fluid Mechanics

Friedrich Ulrich | Chair of Aerodynamics and Fluid Mechanics

High Performance Computing Center Stuttgart (HLRS)

Dr.-Ing. Nadiia Huskova

Jülich Supercomputing Centre (JSC)

Rajveer Saini

Leibniz Supercomputing Centre (LRZ)

Alexander Wellmann



Agenda

- Introduction
- General RDM & FAIR principles in HPMC
- Tools & Systems at LRZ; InHPC-DE
- Break + Survey
- Tools & Systems at JSC
- Tools & Systems at HLRS
- Applications & Best Practices
- Wrap Up / Feedback

Background: Initiatives and networks for RDM

... are everywhere:

Internationally¹⁾

In Europe²⁾

In Germany³⁾

Federal State (e.g. Bavaria)⁴⁾

In Munich⁵⁾

1) <https://www.unesco.org/en/communication-information/open-solutions/open-data>

2) <https://scienceeurope.org/our-priorities/research-data/>

3) https://www.bildung-forschung.digital/digitalezukunft/de/unsere-ueberzeugungen/digitalstrategie-des-bmbf/forschungsdatenmanagement/forschungsdatenmanagement_node.html

4) <https://www.fdm-bayern.org/>

5) <https://forschungsdaten.info/fdm-im-deutschsprachigen-raum/deutschland/bayern/projekte-und-netzwerke/netzwerke/rdmuc-muenchner-arbeitskreis-fuer-forschungsdatenmanagement>

NFDI e.V.

“Nationale Forschungsdateninfrastruktur”

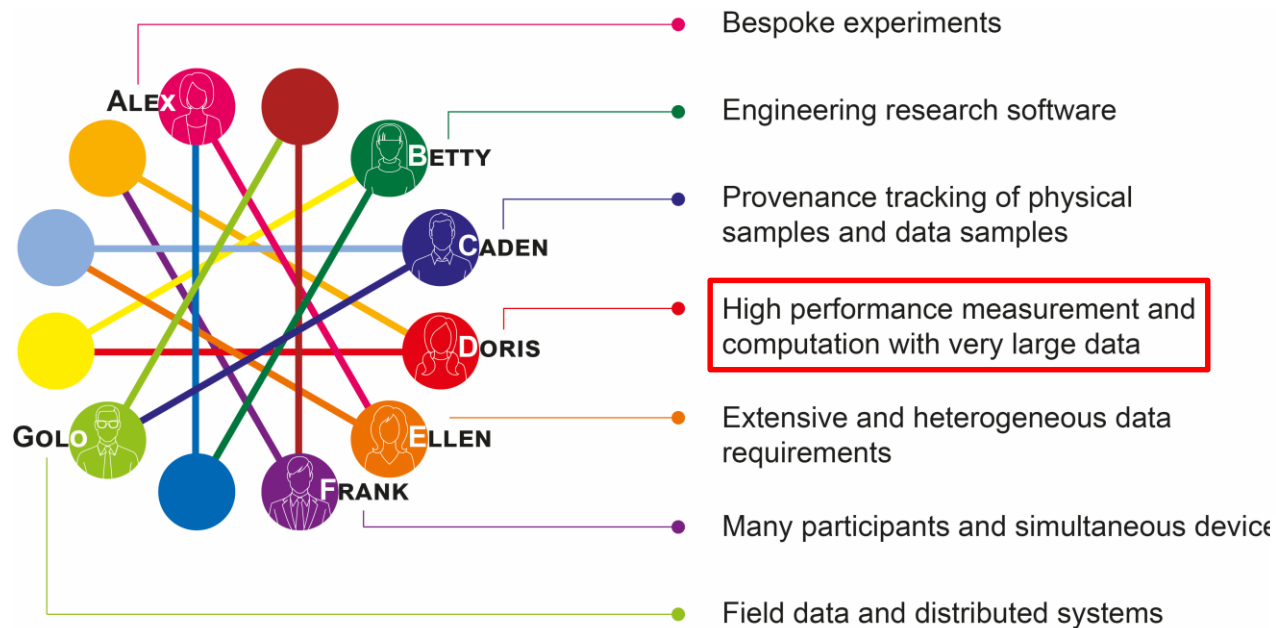
- Registered association funded by the federal government and the federal states (90 Mio. Euro / year)
- Goals:
 - Set **standards** in data management
 - Digital, regional and interconnected **data storage**
 - Enable **innovations and new findings** through available research data
- 26 NFDI consortia will be selected by the German Research Foundation (DFG)
 - e.g. NFDI4Cat, NFDI4Earth, NFDI4CS
 - **NFDI4Ing**



NFDI4Ing

“Nationale Forschungsdateninfrastruktur für die Ingenieurwissenschaften”

- Develop, disseminate, standardize and provide **methods and services** to make engineering research data FAIR



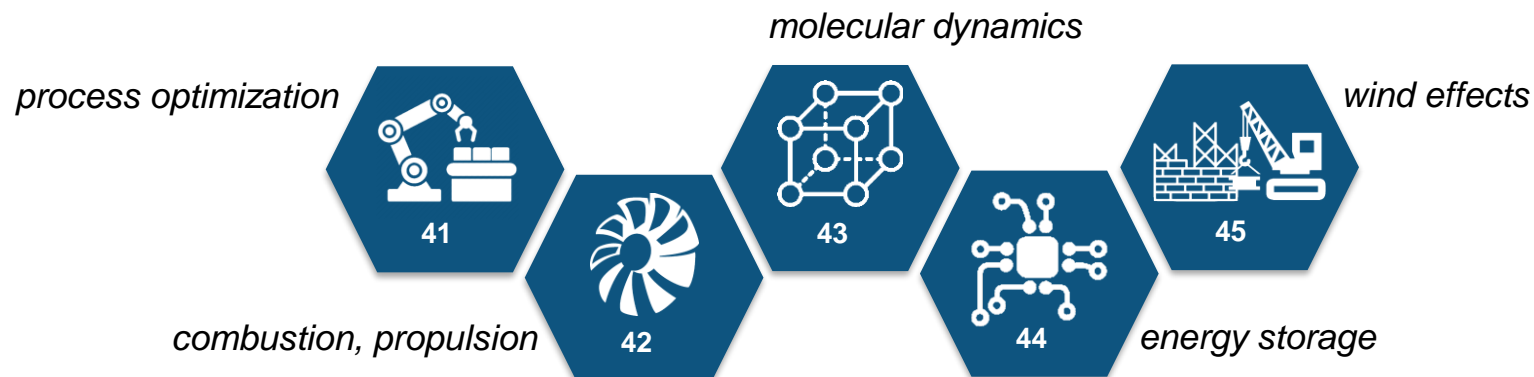
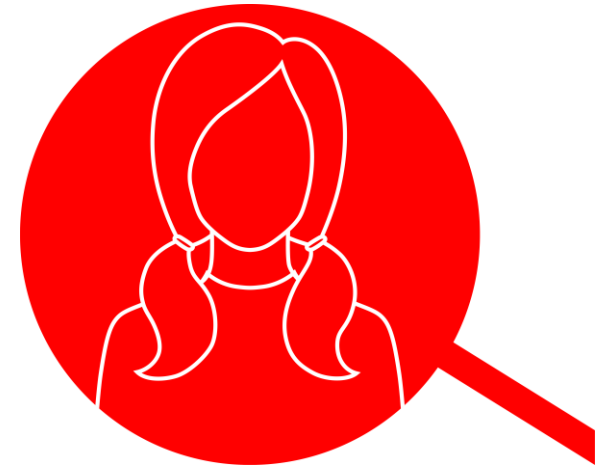
Task Area DORIS DORIS: HPMC

... I'm an engineer conducting and post-processing high-resolution and **high-performance measurements and computation** (simulation) **with very large data** on HPC systems.

The data sets I work with are extremely large and as such are largely immobile. This mandates tailored, hand-made software."

My needs are

- Enable **exchange** of **huge** high-quality **datasets**.
- Provision of HPC-data to foster **wide-spread usage**.
- Drive NFDI-wide **new methodologies** for data sharing

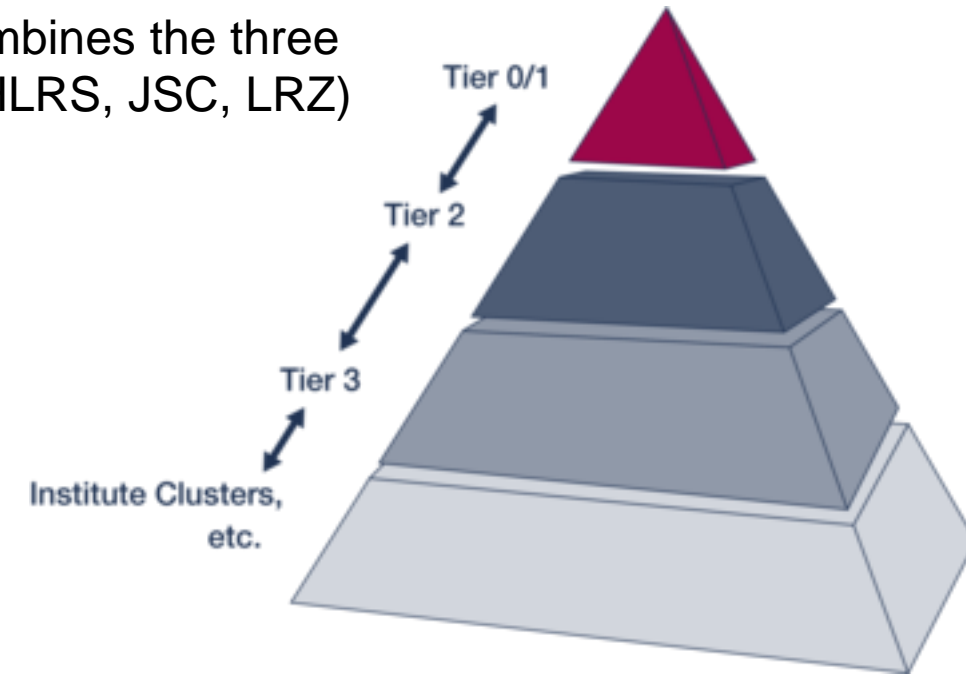


DORIS's patron is
Christian Stemmer

High Performance Measurement and Computing (HPMC)

Focus on tier 0 (EU) / tier 1 (DE)

Gauss Centre for Supercomputing (GCS) combines the three national tier 1 / tier 0 supercomputing centres (HLRS, JSC, LRZ)

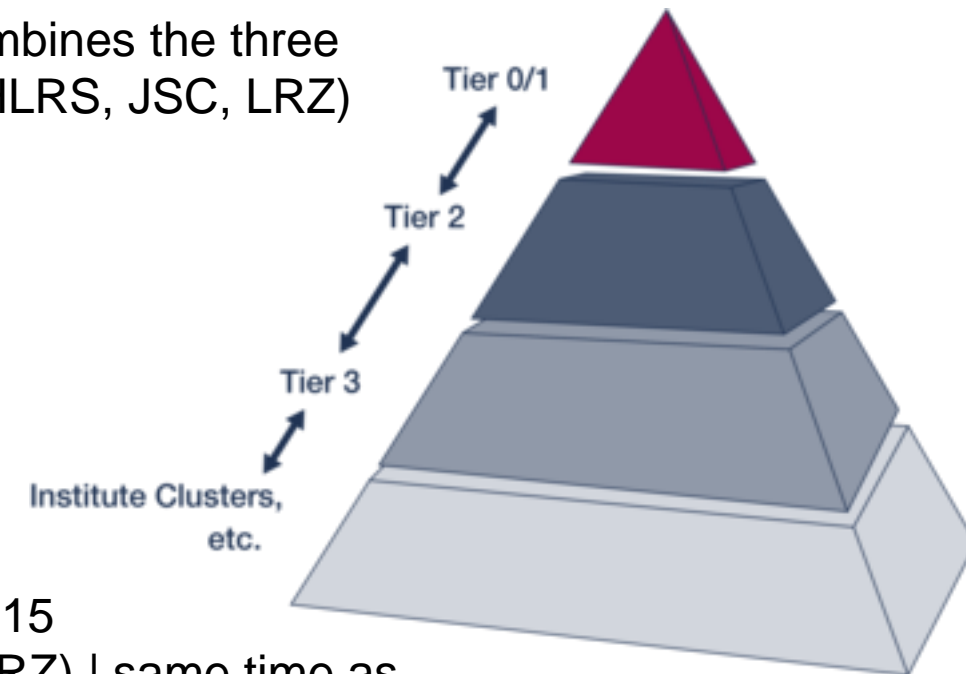


High Performance Measurement and Computing (HPMC)

Focus on tier 0 (EU) / tier 1 (DE)

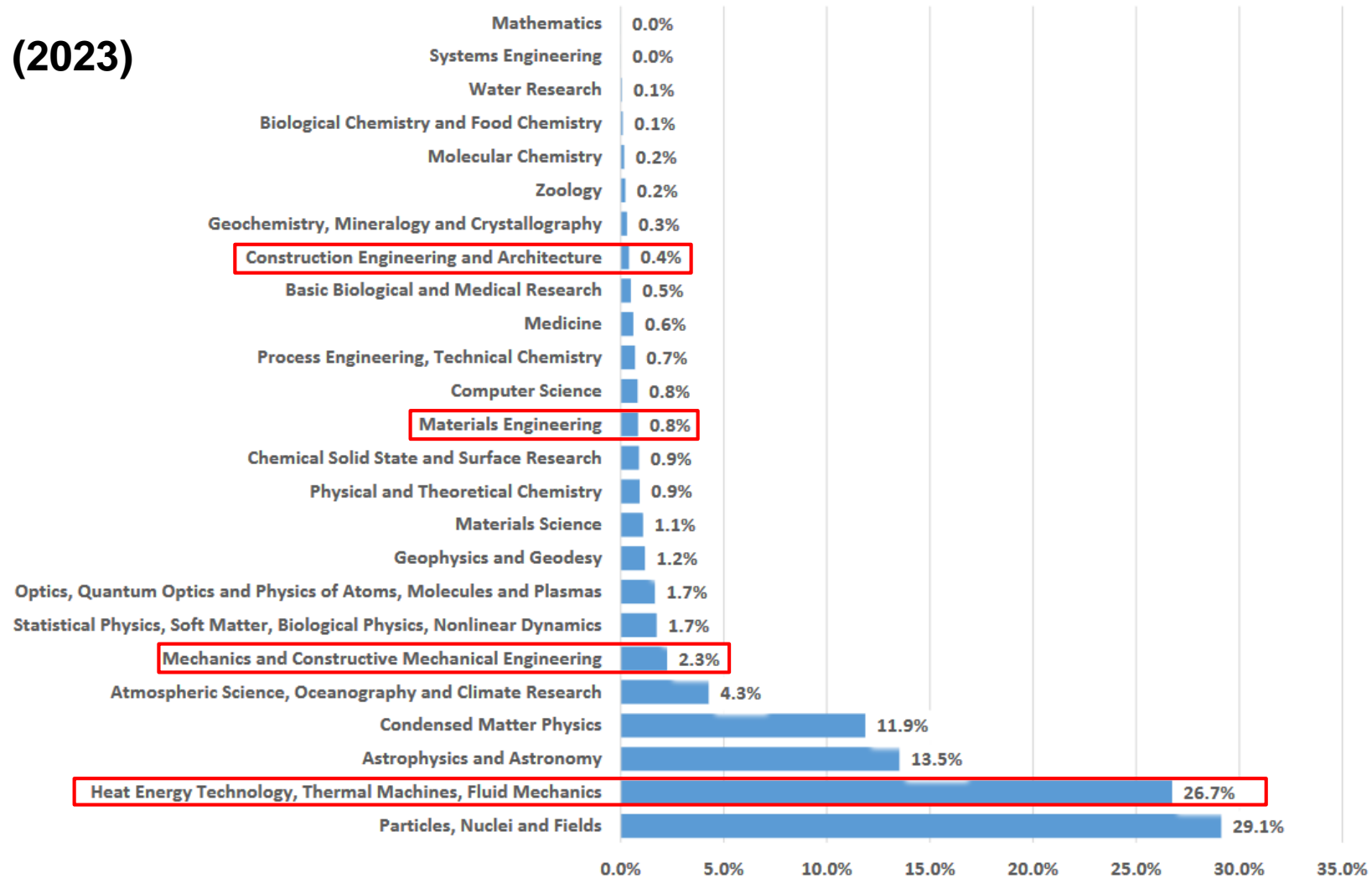
Gauss Centre for Supercomputing (GCS) combines the three national tier 1 / tier 0 supercomputing centres (HLRS, JSC, LRZ)

- Project proposal via GCS required
- Test project: ~300k core hours
 - rolling call, simplified application
- Regular project: ≤ 35 mio core hours
- Large scale project: > 35 mio core hours
 - Peer reviewed
 - Large scale calls: ~July 15 to August 15
 - Regular calls: rolling calls (HLRS & LRZ) | same time as large scale projects (GCS)
- Further information ([link](#)) | application ([link](#))



HPMC: User Statistics

SuperMUC-NG (2023)



https://doku.lrz.de/files/11483092/372441090/6/1712334305907/Statistics-SNG_2023.pdf

What are research data

What are Research Data

Research data are data that are created during a research process or are the result of it

High Performance Measurement

- Tools & methods (!)
- Measurement data
- Metadata (hardware, method etc.)



Analysis and processing of measurement data using HPC

High Performance Computing

- Tools & methods (!)
- Script / code
- Input file, output file, log file
- Raw data, processed data
- Data for secondary research (e.g. energy consumption or temperature in HPC)
- **Metadata**

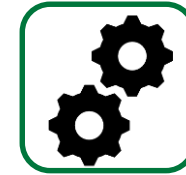
Goal: FAIR Research Data



Findable



Accessible



Interoperable



Reusable

<https://www.go-fair.org/fair-principles/>

HPMC Research Data

Characteristics

- Data are created and stored in personalized accounts directly at HPC centres → no indexing by repositories or search engines
- Special hard- & software required for creating, reading or processing data
- Size: terabyte to petabyte → data is not mobile
- “Data” consists of various components (code, input file, raw data, metadata etc.)
- No established terminology or metadata scheme
- Little best-practice or showcases for research data management

Implementation of FAIR data principles

Findable: storage in personalized accounts, little metadata



Accessible: no access for third parties, insufficient transfer tools



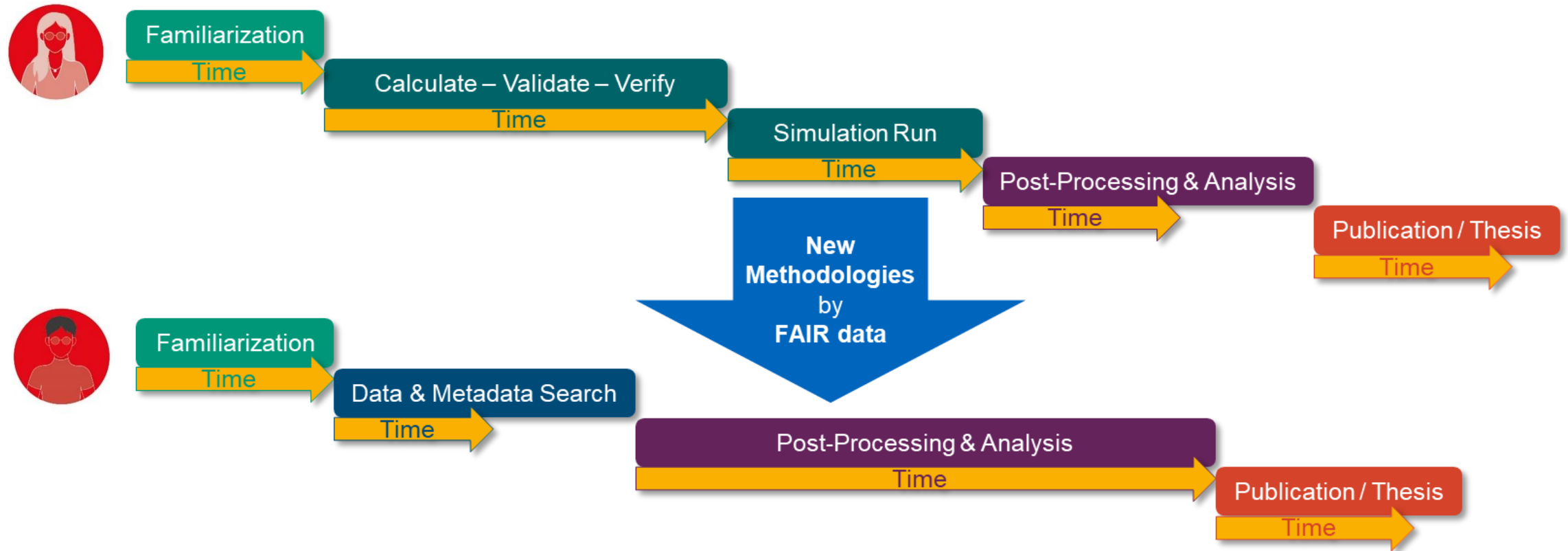
Interoperable: depending on formats and enriched meta



Reusable: computing time at HPC centres required or virtualization (e.g. container)

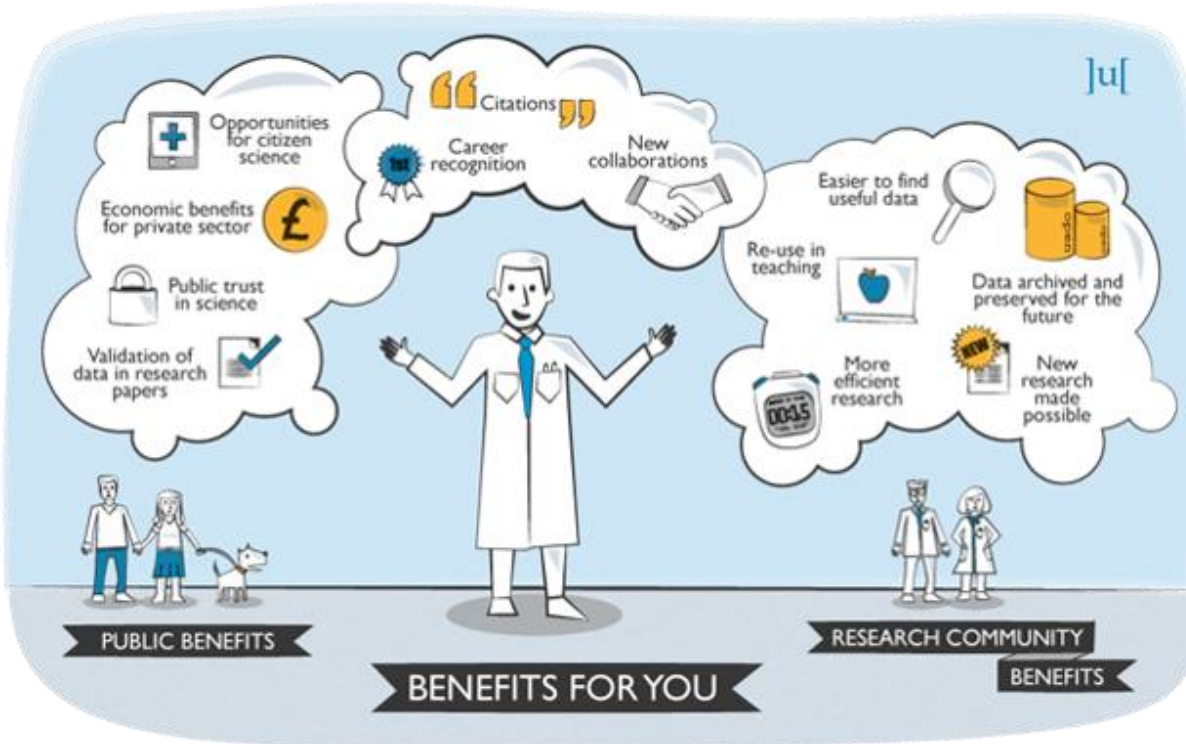


Motivation



Motivation

Why should I invest in research data management?

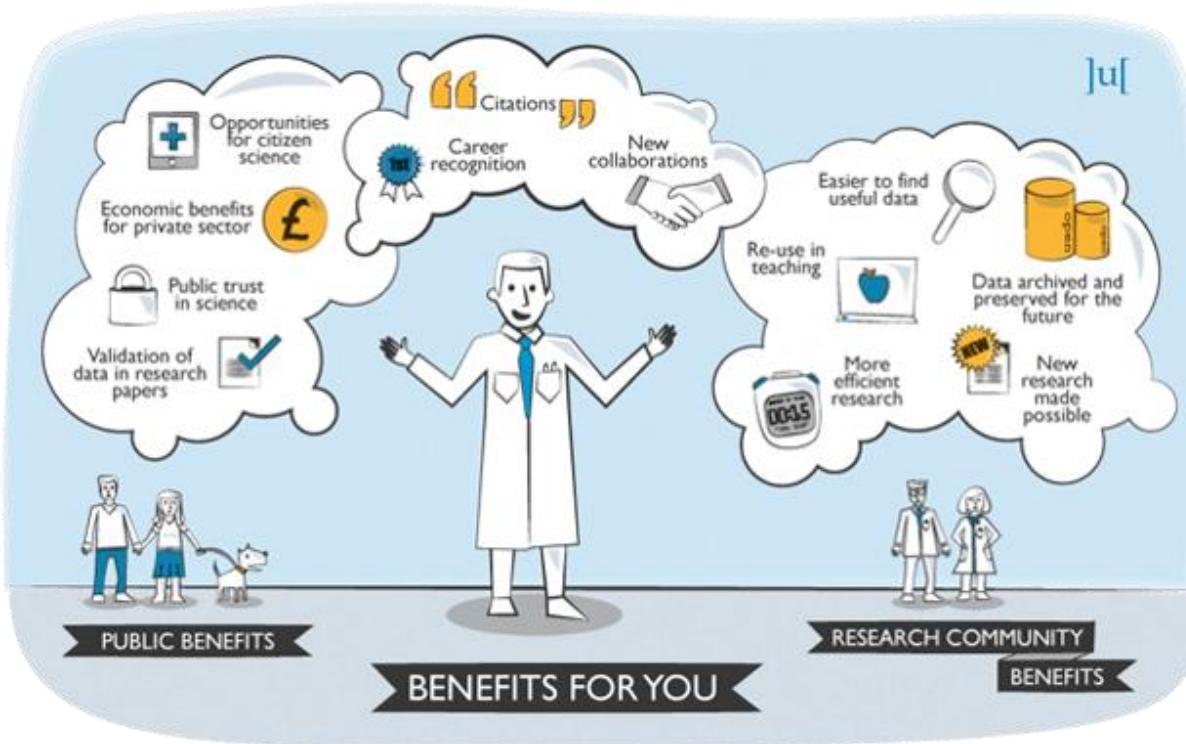


- Scientific integrity and fulfilment of (external) compliance (e.g. DFG)
- Secondary research (e.g. energy consumption or temperature in HPC centres)
- Bookkeeping in your own research, exchange with colleagues in your group and dissemination with external partners, new findings, new methodologies, new workflows, new opportunities by re-using existing data

[<https://www.slideshare.net/brianhole/the-journal-of-open-archaeology-data-and-prime-incentivising-open-data-archiving>]

Motivation

Why should I invest in research data management?



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→ *“do it for yourself”*

[<https://www.slideshare.net/brianhole/the-journal-of-open-archaeology-data-and-prime-incentivising-open-data-archiving>]

Benefits

Extrinsic factors

- Compliance with Good Scientific Practice Principles (e.g. DFG Code of Conduct)
- Compliance with internal guidelines

- Required for access to certain funding streams (e.g. ERC Horizon Europe, from 2024 BMBW/BMBI)
- Increasing political importance (e.g. Federal Data Strategy, NFDI)

- Simplifies re-use by a third party
- Enables secondary research, new findings / methodologies based on FAIR data

- RDM also applies for data from industry projects and proprietary data
 - E.g. access management or deletion deadlines can be controlled by RDM

Benefits

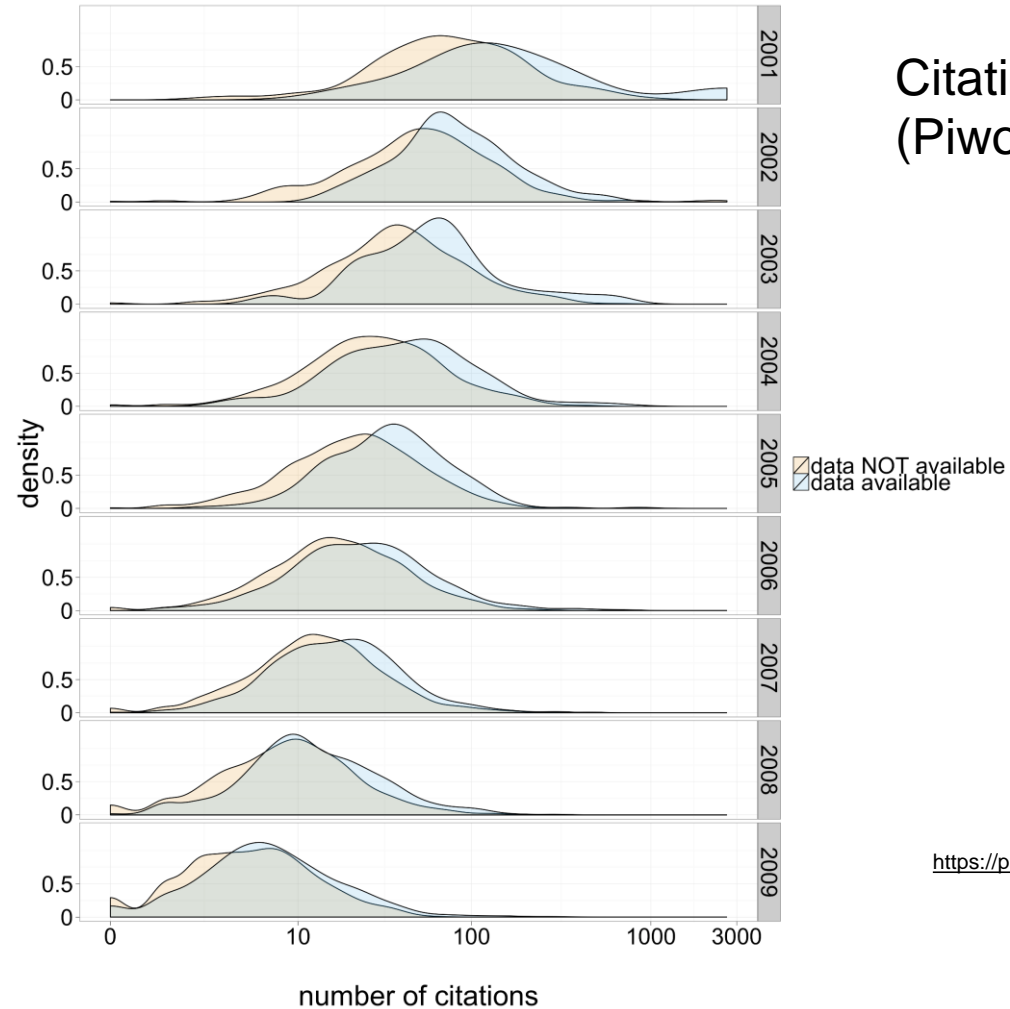
Intrinsic factors

- Simplifies re-use by yourself or your group
- Scientific reputation and transparency
- Visibility and improved odds for collaborations and funding
- New publishing opportunities (e.g. peer reviewed data publishing or data based PhD)
 - Journal “Data in Brief” (Elsevier)
 - NFDI4Ing Journal “ing.grid” (NFDI4Ing)

- Improved project management through RDM
- Minimizes risk of data loss
- Re-use or dissemination of proper data
- „Standing on the shoulder of giants“
 - New findings through (meta-)data analysis
 - Verification and validation of proper models by external data

- Increase of citations by published research data
 - (Publications: 2013, 2016, 2020)

Benefits



Citation density for papers with and without publicly available data
(Piwowar & Vision 2013)

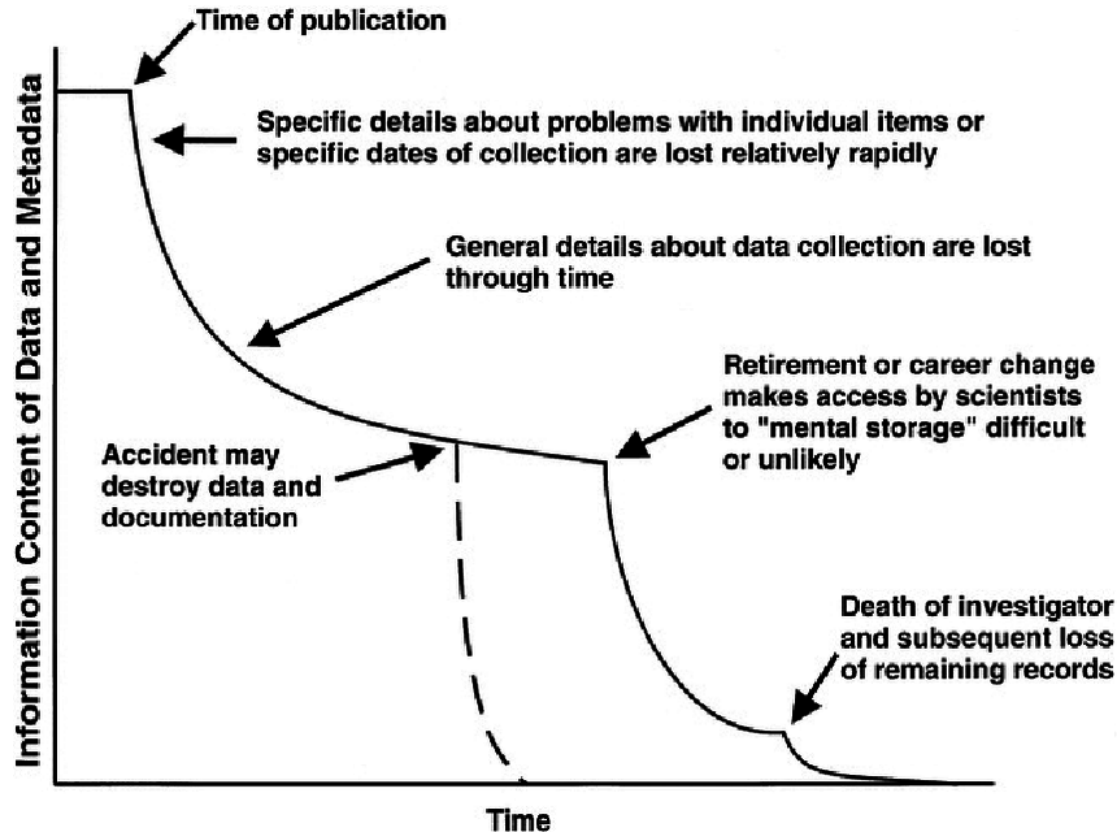
<https://peerj.com/articles/175/> (04.05.2021)

Benefits

Sharing data increases citations (Drachen et al. 2016)

Journal papers published in 2010	Astro-physical Journal (ApJ)	Astronomy and Astrophysics (A&A)	Astronomical Journal (AJ)
All			
# of papers	2501	1918	388
# of citations	74,663	40,829	9465
Mean citations/paper	29.9	21.3	24.4
Datalink papers			
# of papers	794	875	174
# of citations	27,936	22,308	4754
Mean citations/paper	35.2	25.5	27.3
No datalink papers			
# of papers	1707	1043	214
# of citations	46,727	18,521	4711
Mean citations/paper	27.4	17.8	22.0

Benefits



The loss of information about data over time
(Michener et al. 1997)

<https://www.researchgate.net/profile/Adam-Wilson-4/publication/255571027/figure/fig4/AS:297949465726983@1448048096877/Example-of-the-normal-degradation-in-information-content-associated-with-data-and.png> (04.05.2021)

How-to? Follow guidelines

General guidelines (by DFG)



Code of Conduct¹⁾



Handling of Research Data²⁾

Context-specific guidelines



University-specific³⁾



Discipline-specific



Journal-specific



Program-specific

1) <https://doi.org/10.5281/zenodo.6472827>

2) https://www.dfg.de/download/pdf/foerderung/grundlagen_dfg_foerderung/forschungsdaten/guidelines_research_data.pdf

3) <https://web.tum.de/en/researchdata/tum-guidelines/>

How-to? Write a data management plan (DMP)

Draft DMP

Project information, description of existing data, what data (formats, volume), metadata and documentation plan, metadata and data standards, storage and back-up strategy, data sharing, costs

DMP Reuse
Understanding of data
and methods for follow-up
projects



Reuse



Plan



Collect

Update DMP
Document changes of
information in DMP(v1),
methods used, datasets,
responsible researcher



Publish



Process

**Save / Archive and Publish
DMP with Data**



Save

How-to? Cover all relevant aspects in the DMP



Project Administration

- Time
- Costs
- Roles
- ...



Data Characteristics

- Type
- Metadata
- Software
- ...



Data Organisation

- Folders
- File Naming
- Storage
- ...



Ethical & Legal Issues

- Personal Data
- IP
- Contracts
- ...



Preservation & Sharing

- Data Selection
- Repository
- Licenses
- ...

How-to? Estimate costs in your DMP

Consider costs of research data management:

—● **Infrastructure**

(e.g. hardware or software needed to make data reusable)

—● **Personal resources**

(e.g. the position of a data steward or a data manager)

—● **Publication**

(depending on repository, data size, quality checks, data curation)

Check out **funding opportunities** for these costs:

https://www.fdm.uni-hannover.de/fileadmin/fdm/Dokumente/200727_KalkulationFDMKosten.pdf

How-to? Use tools and templates for DMPs

RDMO <https://rdmorganiser.github.io/en>

German tool developed in a DFG project; discipline-specific templates available

DMP-Toolguide <https://zenodo.org/record/4632308#.YkV4ONNBw2w>

List of software tools for DMPs

DMPonline <https://dmponline.dcc.ac.uk>

British tool, suitable for applications to British and European research funding agencies

DMPTool <https://dmptool.org>

US-American tool, suitable for applications to American research funding

DSW <https://ds-wizard.org/>

European tool (developed in the Netherlands and Czech Republic)

DFG Checklist https://www.dfg.de/research_data/checklist

mandatory for all DFG projects since March 2022

(https://www.dfg.de/en/research_funding/announcements_proposals/2022/info_wissenschaft_22_25/index.html)

HPC template by TUM & LRZ <https://zenodo.org/record/5801838#.YjSN0DUxmUk>

Basic template (~ 1h required)

Feedback? (new version planned)

Metadata

Data about data

- Key elements of documentation
- Stored independently or in combination with the data they describe
- Ideally standardized
- Ideally human and machine-readable
- **Increased findability and interoperability by using standardized metadata vocabulary**



```
2022/08/22  
Baljit Singh/  
Manuela Lannister/  
Olgiard Nolte  
4035/8885/349/  
Edge-Fractile-Ten-  
sile-Test  
/2022/02/04  
ISSN:4567-9283  
DOI:10.14459/2021m  
d1635091  
...
```

Store metadata – but about which data?

General:

- Title, location, creator name, description, data collection, ...

Raw data:

- Obtained by whom, using restrictions (for certain project only, (not) publish), content information (where, which methods – sampling, parameter analysing), devices, column names, units

Processed data:

- Creator of file, script for file production, time of creation, which input data (raw, pre-processed, interconnection of files), methods used, used software or packages, relationship between data

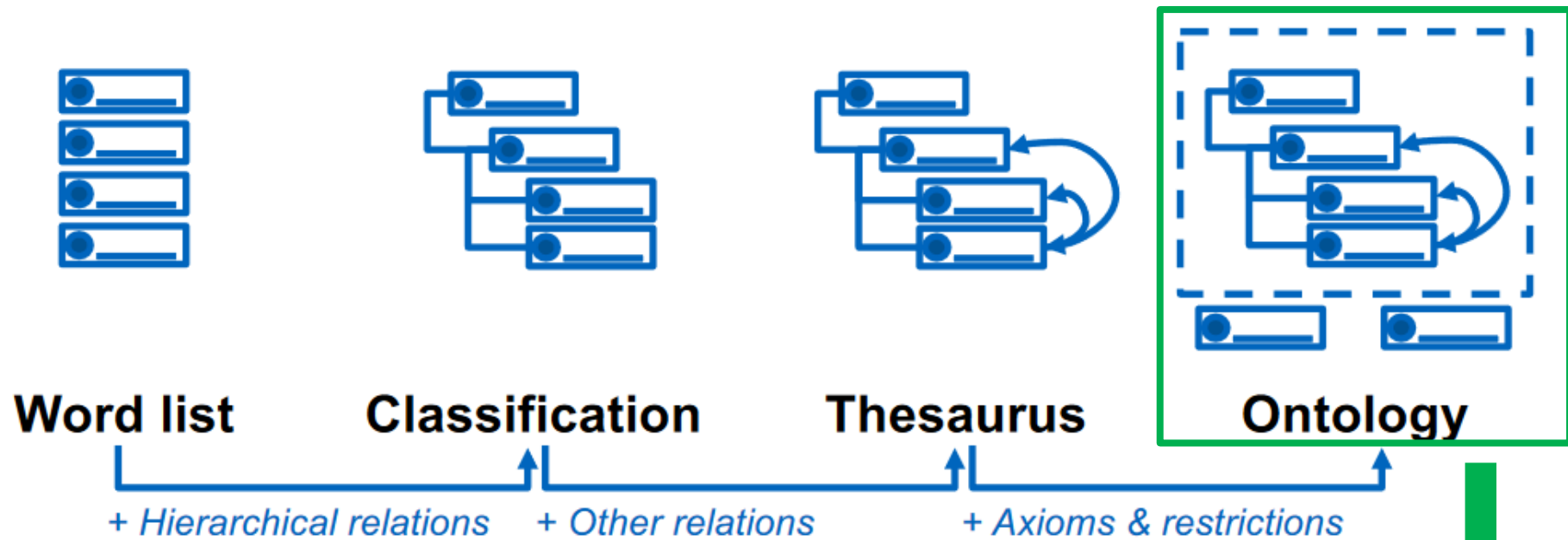
Programming scripts:

- Script functions, creator of script, usage of script

Source: Sonnenberg, Hauke; Rustler, Michael; Sprenger, Christoph (2019) Best Practices in Research Data Management, <https://kwb-r.github.io/fakin.doc/index.html>

Standardized Metadata: Controlled Vocabularies

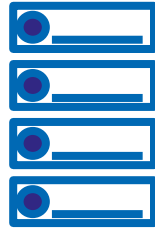
„Data about data“



Adapted from 2019-09-26_Metadata TU9 Treffen Darmstadt

- **Findability**
- **Interoperability**
- **AI & Machine Learning**
- *Human readable?*

Standardized Metadata: Controlled Vocabularies

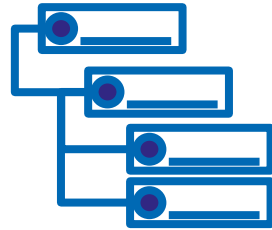


Word list

- Definitions
- Consistent choice of words

R Radiobiology: Study of ionizing radiation and its interactions with human beings
S Structural Biology: Study of the structure of biological molecules Soil Biology: Study of living organisms in the soil Systems Biology: Study of biological systems
T Taxonomy: Study of naming, classifying, arranging, and describing living organisms
V Virology: Study of viruses as well as virus diseases
Z Zoology: Study of the plant kingdom

Standardized Metadata: Controlled Vocabularies



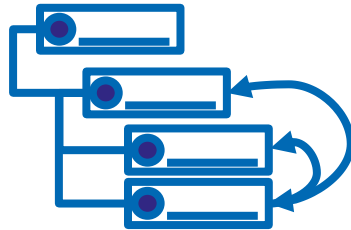
Classification

- Word list + hierarchy
- Easier search
- Easier analysis of information

Body Regions [A01] -

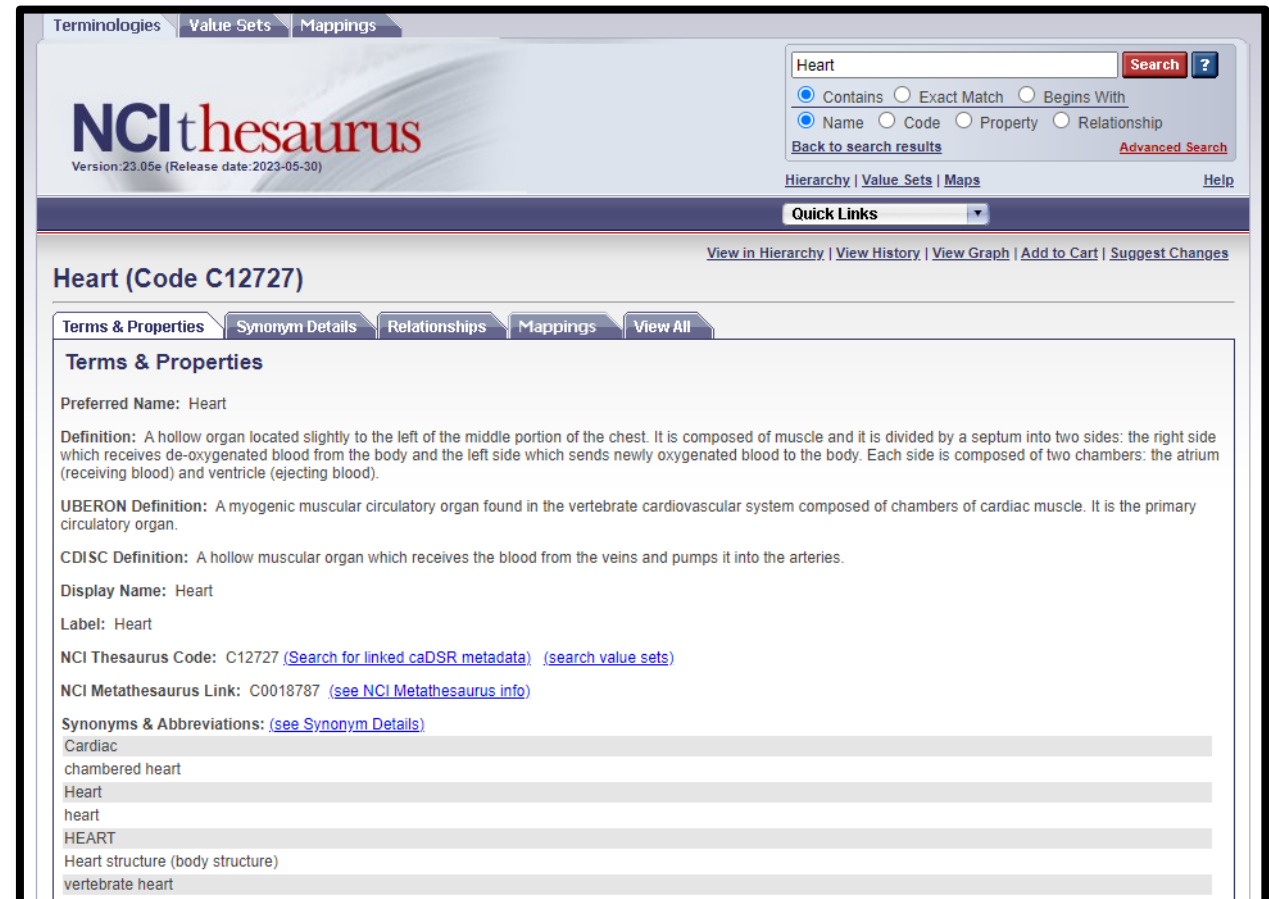
- Anatomic Landmarks [A01.111]
- Breast [A01.236] +
- Extremities [A01.378] +
- Head [A01.456] +
- Neck [A01.598] +
- Organs at Risk [A01.635]
- Perineum [A01.719]
- Torso [A01.923] -
 - Abdomen [A01.923.047] -
 - Abdominal Cavity [A01.923.047.025] -
 - Peritoneum [A01.923.047.025.600] -
 - Douglas' Pouch [A01.923.047.025.600.225]
 - Mesentery [A01.923.047.025.600.451] +
 - Omentum [A01.923.047.025.600.573]
 - Peritoneal Cavity [A01.923.047.025.600.678]
 - Peritoneal Stomata [A01.923.047.025.600.700]
 - Retroperitoneal Space [A01.923.047.025.750]

Standardized Metadata: Controlled Vocabularies



Thesaurus

- Classification + relationship
- Better description of topic



Terminologies Value Sets Mappings

Heart ?

Contains Exact Match Begins With

Name Code Property Relationship

[Back to search results](#) [Advanced Search](#)

[Hierarchy](#) | [Value Sets](#) | [Maps](#) [Help](#)

Quick Links

[View in Hierarchy](#) | [View History](#) | [View Graph](#) | [Add to Cart](#) | [Suggest Changes](#)

Heart (Code C12727)

Terms & Properties Synonym Details Relationships Mappings View All

Terms & Properties

Preferred Name: Heart

Definition: A hollow organ located slightly to the left of the middle portion of the chest. It is composed of muscle and it is divided by a septum into two sides: the right side which receives de-oxygenated blood from the body and the left side which sends newly oxygenated blood to the body. Each side is composed of two chambers: the atrium (receiving blood) and ventricle (ejecting blood).

UBERON Definition: A myogenic muscular circulatory organ found in the vertebrate cardiovascular system composed of chambers of cardiac muscle. It is the primary circulatory organ.

CDISC Definition: A hollow muscular organ which receives the blood from the veins and pumps it into the arteries.

Display Name: Heart

Label: Heart

NCI Thesaurus Code: C12727 ([Search for linked caDSR metadata](#)) ([search value sets](#))

NCI Metathesaurus Link: C0018787 ([see NCI Metathesaurus info](#))

Synonyms & Abbreviations: ([see Synonym Details](#))

Cardiac

chambered heart

Heart

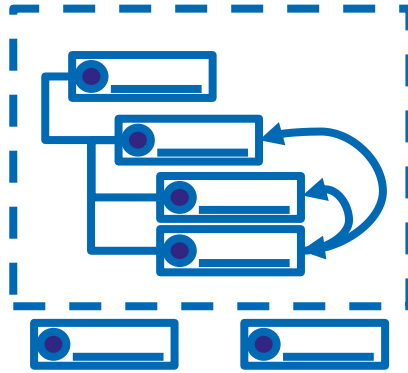
heart

HEART

Heart structure (body structure)

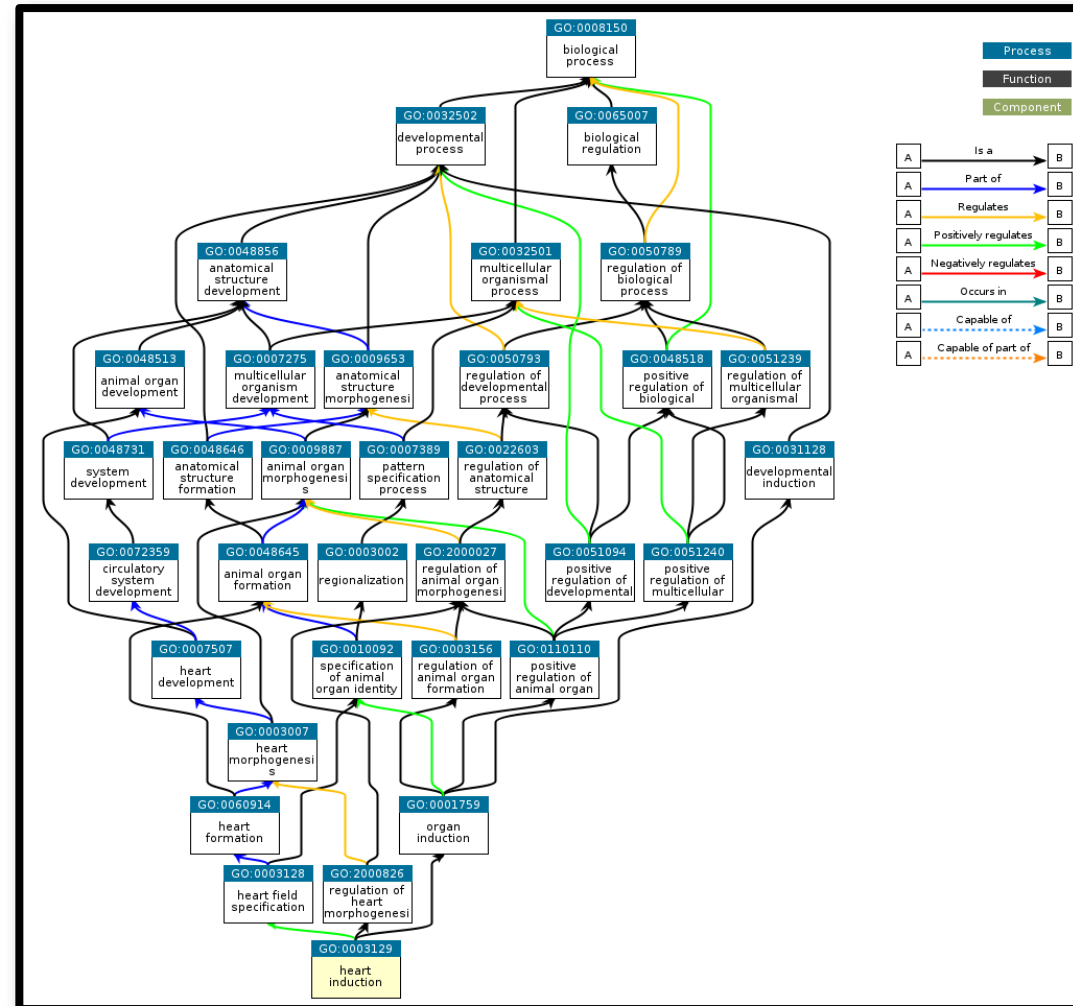
vertebrate heart

Standardized Metadata: Controlled Vocabularies



Ontology

- Thesaurus + assumptions + restrictions
- Formal and digital exchange of knowledge



Metadata: Standardized Schemes

Scheme	URL	Purpose / Domain
NASA Thesaurus	https://www.sti.nasa.gov/docs/thesaurus/thesaurus-vol-1.pdf	Aerospace
PhySH	https://physh.org/browse	Physics
DataCite	https://schema.datacite.org/ https://dhvlab.gwi.uni-muenchen.de/datacite-generator/	Publication and citation of research outputs Metadata Generator
DublinCore	https://www.dublincore.org/specifications/dublin-core/dcmi-terms/	Documents and digital objects
CodeMeta	https://codemeta.github.io/terms/	Software
DCAT	https://www.w3.org/TR/vocab-dcat-3/	Description of data sets
EngMeta	https://darus.uni-stuttgart.de/file.xhtml?persistentId=doi:10.18419/darus-500/3&version=1.0	Metadata scheme for engineering science
Metadata4Ing	https://nfdi4ing.pages.rwth-aachen.de/metadata4ing/metadata4ing/index.html	Ontology for engineering science

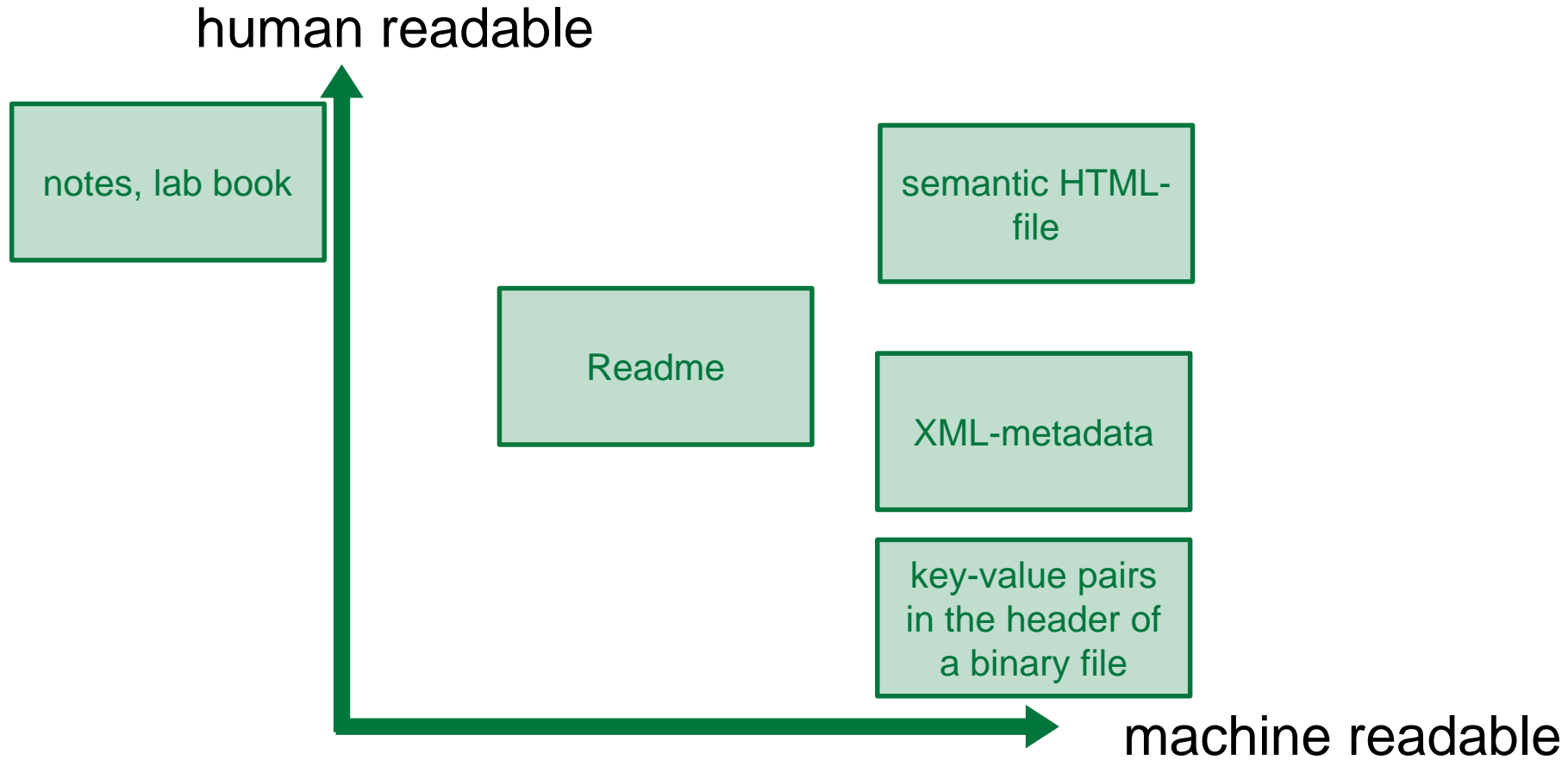
- **NFDI4Ing Terminology Service:** <https://terminology.nfdi4ing.de/ts/>
- **Research Data Alliance Metadata Standards Directory:** <http://rd-alliance.github.io/metadata-directory/>
- **Ontobee Ontology Server:** <https://www.ontobee.org/>
- **Vocabulary finder:** <https://schema.org/>

Metadata: Standardized Schemes

Scheme	URL	Purpose / Domain
NASA Thesaurus	https://www.sti.nasa.gov/docs/thesaurus/thesaurus-vol-1.pdf	Aerospace
PhySH	https://physh.org/browse	Physics
DataCite	https://schema.datacite.org/ https://dhvlab.gwi.uni-muenchen.de/datacite-generator/	Publication and citation of research outputs Metadata Generator
DublinCore	https://www.dublincore.org/specifications/dublin-core/dcmi-terms/	Documents and digital objects
CodeMeta	https://codemeta.github.io/terms/	Software
DCAT	https://www.w3.org/TR/vocab-dcat-3/	Description of data sets
EngMeta	https://darus.uni-stuttgart.de/file.xhtml?persistentId=doi:10.18419/darus-500/3&version=1.0	Metadata scheme for engineering science
Metadata4Ing	https://nfdi4ing.pages.rwth-aachen.de/metadata4ing/metadata4ing/index.html	Ontology for engineering science

including workflow based **HPMC-subontology!**  GitLab

Metadata: Schemes





<http://doi.org/10.5281/zenodo.2660187>

Checklist: Metadata for FAIR Data

- **Findable**
 - Data is described with metadata ✓
 - Metadata is indexed ✓
 - Metadata and data are linked ✓
- **Accessible**
 - Metadata can be accessed via standardized (open, free) protocol (with authentication if necessary) ✓
- **Interoperable**
 - Metadata use formal, accepted language and formats ✓
 - Metadata use controlled vocabularies ✓
- **Reusable**
 - Metadata determine which use is permitted (license) ✓
 - Metadata describe the creation of the data (provenance) ✓
 - Metadata describe the data sufficiently and according to professional standards ✓


Best Practice for Metadata Publication


Detail View


m-AIA Dataset  

Data format	x
Reynolds number	x
Mach number	x
Dimensions	x
Solver	x
Created on	x
Creator	x
Computed on machine	x

Field Properties


Term IRI 

Term IRI 


Field Name 

Field Name de


Field Name en

Minimum Required Entries 


Minimum Required Entries

Maximum Possible Entries 


Maximum Possible Entries

Position On Metadata Form 

Position On Metadata Form

Property Type 

Datatype

Datatype 

-- Please select an option --

Show String-based Properties

Show Value-based Properties

Show Administrative Properties



Data publication: Choosing a repository

Types of repositories:

generic



discipline-specific



PANGAEA.



DaRUS

gesis
Leibniz-Institut
für Sozialwissenschaften

media-specific



TIB AV-PORTAL

institutional

MEDIATUM

Repositories / publishing
opportunities at HPC centres

Check out:

- Terms of use
- Size limit for a dataset
- Only EU specific or worldwide spread
- FAQs Section

Data publication: Choosing a repository

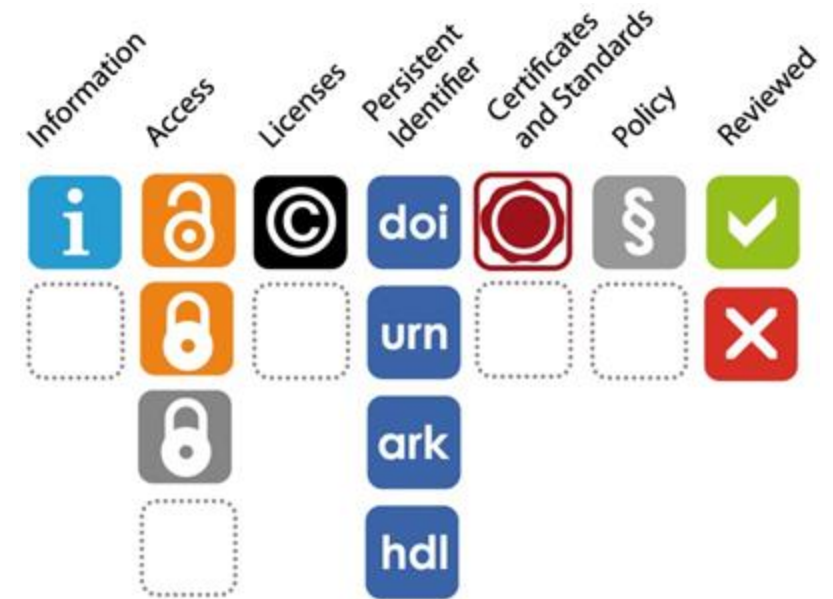
re3data.org
REGISTRY OF RESEARCH DATA REPOSITORIES

<https://www.re3data.org/>

<https://repositoryfinder.datacite.org/>


Filter by

- Subject
- Content type
- Country
- Certificates
- Data access
- Licenses
- Keywords
- Metadata standards
- ...



https://www.forschungsdaten.org/images/7/73/Re3data_icons.jpg

Data publication: Digital Object Identifier (DOI)

- Most prominent persistent identifier in science
- Managed by the International DOI Foundation (<http://www.doi.org/>)
- Usable for
 - Papers
 - Data
 - **Software (!)**
- Makes data citable
 - suggestions for citation styles: <https://www.dcc.ac.uk/guidance/how-guides/cite-datasets>
- **Concept DOI**
 - Enables versioning, e.g.: <https://mediatum.ub.tum.de/1694401>
 - Also applicable for Git-repositories: https://gitlab.lrz.de/nfdi4ing/crawler/-/blob/master/CITATION.cff?ref_type=heads
 - Recommendation: (e.g. [CITATION.cff](#)) with Concept DOI  GitLab



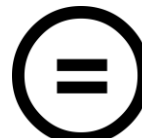
Data publication: Licences



Attribution (BY)
Credit must be given to the creator



Non-commercial (NC)
Only noncommercial uses of the work are permitted

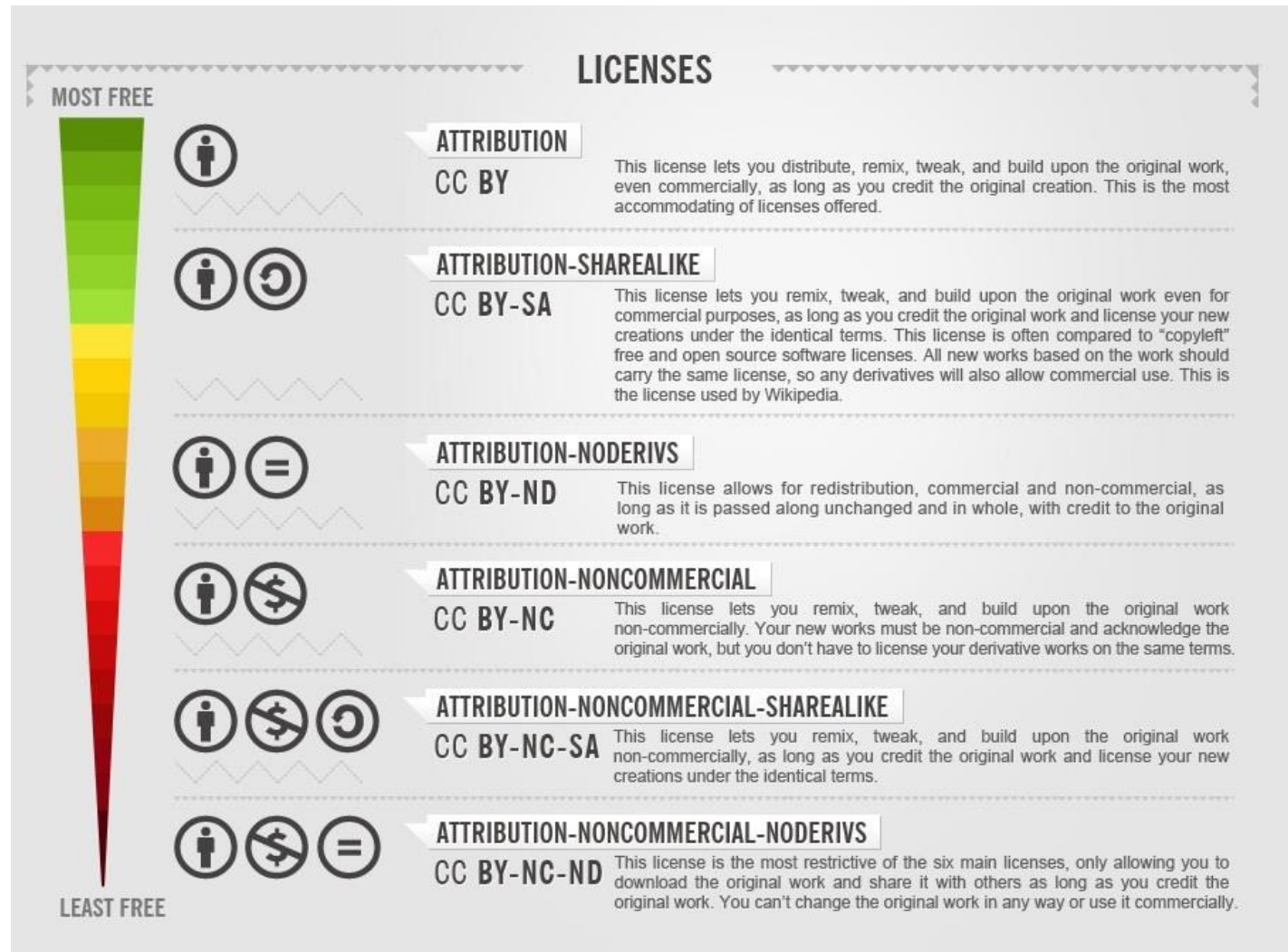


No derivative works (ND)
No derivatives or adaptations of the work are permitted

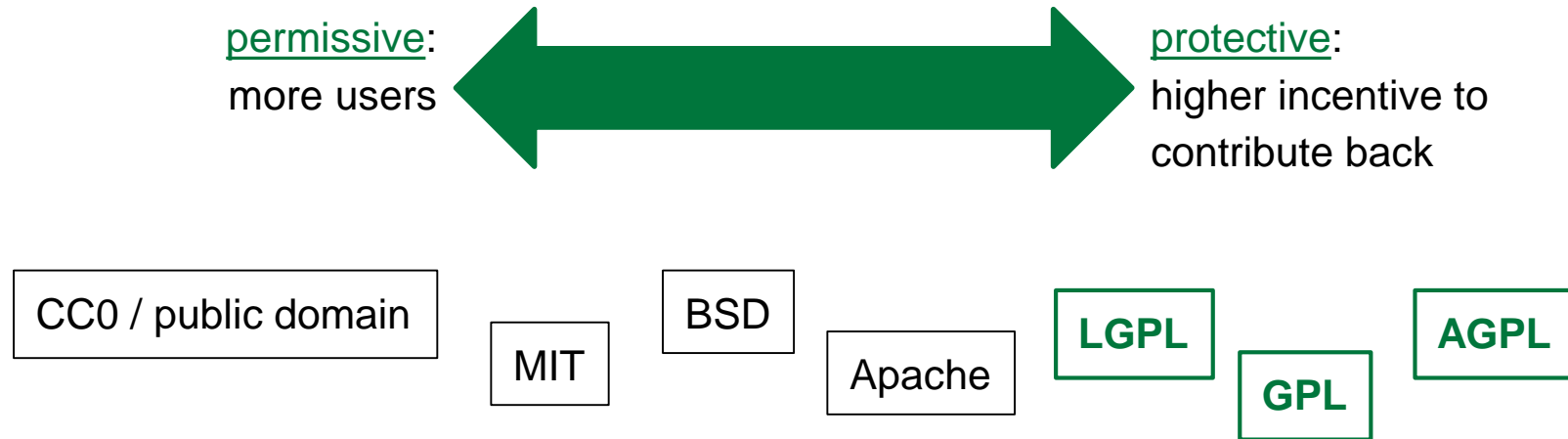


Share-alike (SA)
Adaptations must be shared under the same terms

Data publication: Licences



Data publication: Software licences



Further information:

<https://mediatum.ub.tum.de/doc/1289704/4>, <https://choosealicense.com/>

Data publication: Licences

Keep in mind:

- Usually the more restrictive license prevails
- Not all combinations are possible!
- Check the license version
- Check the **license compatibility** first if you work with data from other people:
<https://joinup.ec.europa.eu/collection/eupl/solution/joinup-licensing-assistant/jla-compatibility-checker>

Data publication: Formats

Text	PDF/A <i>no format</i> : TXT <i>editable</i> : ODT, RTF, HTML <i>formulas</i> : LaTeX (TEX)
Table	CSV, TSV HDF5 (numerical data)
Visualizations	<i>Raster</i> : PNG, TIFF <i>Vector</i> : SVG, EPS
Multimedia	<i>Container</i> : MKV, WebM, OGG <i>Video-Codec</i> : AV1, VP9 <i>Audio-Codec</i> : FLAC, WAV, Vorbis, Opus
Data base	SIARD, Dump, XML
structured data	XML, JSON, YAML (metadata)

<https://www.forschungsdaten.info/themen/bewahren-und-nachnutzen/formate-erhalten/>

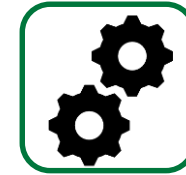
Goal: FAIR Research Data



Findable



Accessible



Interoperable



Reusable

<https://www.go-fair.org/fair-principles/>

Goal: FAIR Research Data

FAIRness check:

ARDC

Questionnaire

[https://ardc.edu.au/res
ource/fair-data-self-
assessment-tool/](https://ardc.edu.au/resource/fair-data-self-assessment-tool/)

DANS

Questionnaire

[https://fairaware.dans.k
naw.nl/](https://fairaware.dans.knaw.nl/)

FAIRsFAIR

Metrics

[https://doi.org/10.5281/
zenodo.4081213](https://doi.org/10.5281/zenodo.4081213)

FAIRsFAIR

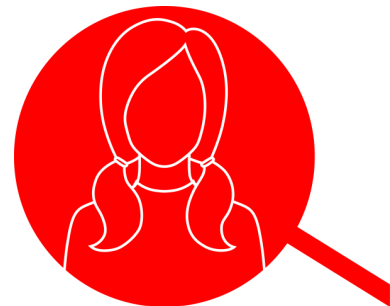
F-UJI Tool

<https://www.f-uji.net/>

Information and Links

Downloads

- **Slides, publications** etc.: <https://zenodo.org/communities/nfdi4ing?page=1&size=20>
- **DORIS' Software**: <https://gitlab.lrz.de/nfdi4ing>
- **Data Management Plan - HPMC-template**: <https://zenodo.org/record/5801838#.YjSN0DUxmUk>
- **Metadata4Ing Ontology** for Workflows in (Engineering) Science
 - Documentation: <https://nfdi4ing.pages.rwth-aachen.de/metadata4ing/metadata4ing/index.html>
 - GitLab: <https://git.rwth-aachen.de/nfdi4ing/metadata4ing/metadata4ing>
 - Publication: <https://zenodo.org/record/5957104#.ZBxm5M7MKUk>
 - Preprint on HPMC subontology: <https://preprints.inggrid.org/repository/view/12/>
- **Handreichung zu rechtlichen Aspekten** des Forschungsdatenmanagements: <https://mediatum.ub.tum.de/1690463>



Outlook

Events

- Fall 2024 (tbd): **On site Workshop Research Data Management for Science and Engineering at TUM** (for PhD-students); announcement within summer (<https://www.docgs.tum.de/>).
- 18. & 19. September 2024: **NFDI4ing Conference** (online): <https://nfdi4ing.de/?p=21237>

Links & Contact

- **Newsletter:** https://lists.tu-darmstadt.de/mailman/listinfo/nfdi4ing_taskarea_doris
- Mail: info-doris@nfdi4ing.de (confirmation of participation needed?)
- Web: <https://nfdi4ing.de/archetypes/doris/>

Call for Contributions

- ing.grid - the new open access journal for FAIR Data Management: <https://www.inggrid.org/>
- **Pilot users & use cases:**
 - Compute Cloud Server
 - Metadata Schema & Metadata Crawling



<https://www.flaticon.com/de/kostenlose-icons/idee> Idee Icons erstellt von Freepik - Flaticon

Further Information

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*The authors gratefully acknowledge the **Gauss Centre for Supercomputing** e.V. (www.gauss-centre.eu) for funding this project by providing computing time through the John von Neumann Institute for Computing (NIC) on the GCS Supercomputer **JUWELS[1] at Jülich Supercomputing Centre (JSC)**. [1] Jülich Supercomputing Centre. (2021). JUWELS Cluster and Booster: Exascale Pathfinder with Modular Supercomputing Architecture at Juelich Supercomputing Centre. *Journal of large-scale research facilities*, 7, A183. <http://dx.doi.org/10.17815/jlsrf-7-183>*

Further Information

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Katja Kessler	TUM: University Library Research Service Centre
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Prof. Christian Stemmer	TUM: Chair of Aerodynamics and Fluid Mechanics
Sonja Thielen	TUM: University Library Research Service Centre
Friedrich Ulrich	TUM: Chair of Aerodynamics and Fluid Mechanics

Coffee Break

The workshop will continue at **11:42**

Please take the time to fill out our **survey on reproducibility and postprocessing** in high performance computation (link is in the chat):

<https://collab.dvb.bayern/display/TUMrdm/Survey:+Reproducibility+and+Postprocessing+i+n+HPC>



[https://www.flaticon.com/de/kostenlose-
icons/idee](https://www.flaticon.com/de/kostenlose-icons/idee) Idee Icons erstellt von Freepik -
Flaticon