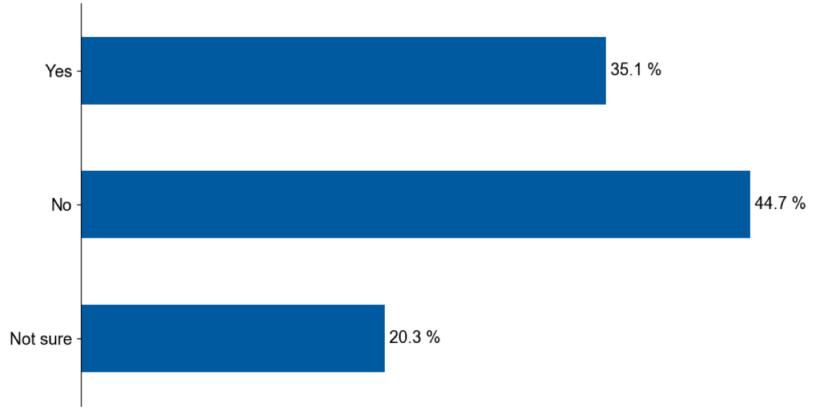
# **Recent Survey on RDM Practices**



https://oceanrep.geomar.de/id/eprint/57494/



**Figure 14: "Do you document your research data in a structured way?** (e.g., using forms, templates or schemas)". (Single choice question, available to all respondents, number of respondents who answered this question: n = 582, relative amounts refer to n)

With massive "thanks" to M. Demleitner, H. Enke, P. Fuhrmann, A. Geiser, G. Günther, A. Haungs, M. Köhler, O. Mannix, S. Servan, C. Wissing + others!



Thomas Schörner (DESY)

JENA Computing Workshop

Bologna, 12-14 June 2023

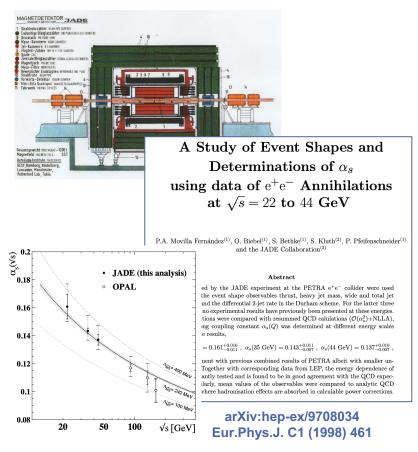






# Introduction Data Preservation, FAIR Principles etc.

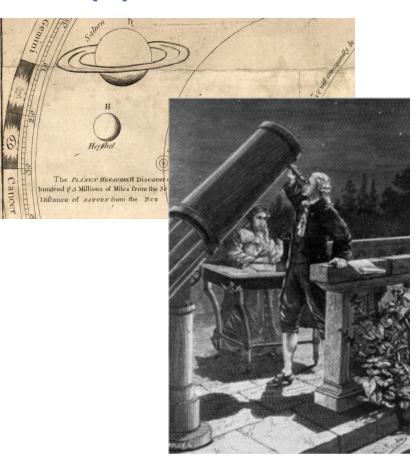
# Instead of an Introduction (1)

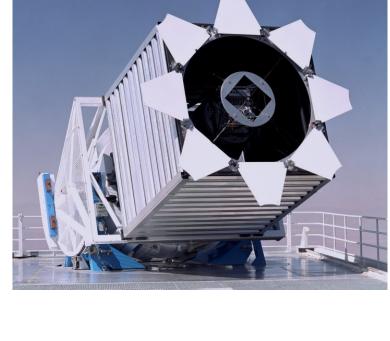


JADE experiment at DESY's PETRA e+e-collider (1979-86) E.g. discovery of three-jet events → gluon discovery

Re-use and re-interpretation 

new insights!





Herschel's discovery of Uranus: It is a not a star, and discovery of Neptune!

Interpretation in light of new discoveries

→ far-reaching conclusions.

SDSS designed to determine beta parameter, focus on galaxies. Later numerous discoveries concerning stars.

New by-product results that enter the focus only later.

## Instead of an Introduction (2): ZEUS and DPHEP

International Conference on Computing in High Energy and Nuclear Physics 2012 (CHEP2012) IOP Publishing Journal of Physics: Conference Series **396** (2012) 022033 doi:10.1088/1742-6596/396/2/022033

#### **Data Preservation in High-Energy Physics**

Study Group for Data Preservation and

DPMEP Long Term Analysis in High Energy Physics

http://dphep.org













#### The ZEUS data preservation project

Janusz Malka and Katarzyna Wichmann on behalf of the ZEUS collaboration

Deutsches Elektronen-Synchrotron, Notkestr 85, 22607 Hamburg, Germany

E-mail: janusz.malka@desy.de,katarzyna.wichmann@desy.de

Abstract. A project to allow long term access and physics analysis of ZEUS data (ZEUS data preservation) has been established in collaboration with the DESY-IT group. In the ZEUS approach the analysis model is based on the Common Ntuple project, under development since 2006. The real data and all presently available Monte Carlo samples are being preserved in a flat ROOT ntuple format. There is ongoing work to provide the ability to simulate new, additional Monte Carlo samples also in the future. The validation framework of such a scheme using virtualisation techniques is being explored. The goal is to validate the frozen ZEUS software against future changes in hardware and operating system. A cooperation between ZEUS, DESY-IT and the library was established for document digitisation and long-term preservation of collaboration web pages. Part of the ZEUS internal documentation has already been stored within the HEP documentation system INSPIRE. Existing digital documentation, needed to perform physics analysis also in the future, is being centralised and completed.

**Table 1.** The DPHEP preservation modes listed in order of increasing complexity.

Table 1. The Di HEI preservant	on modes fisted in order of increasing complexity.
Preservation Model	Use Case
1. Additional information	Publication related information
2. Provide data in simplified format	Outreach, training
3. Preserve the analysis level	Full scientific analysis possible,
software and data format	based on existing reconstruction
4. Preserve the full simulation and	Retain the full potential of the experimental data
reconstruction software as well	
as the basic level data	

dphep.org, arXiv:0912.0255

One important conclusion: Computers and storage alone (today: federated computing) are not enough; software and (meta)data management are as important.

# Instead of an Introduction (3): The FAIR Principles

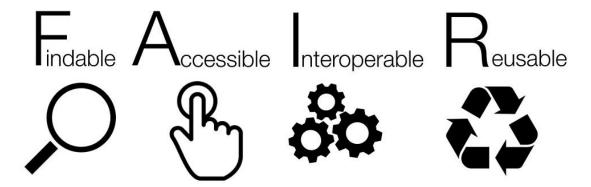
Encountering problems

to find data

to access data

to understand data

to (re)use data



## SCIENTIFIC DATA 1101101 OIL 110110 OIL 11010 OIL 11010 OIL 11010 OIL 11010 OIL 11010 OIL 110110 OIL 110110 OIL 1101

Amended: Addendum

#### OPEN

SUBJECT CATEGORIES

» Research data

» Publication

characteristics

#### Comment: The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson et al.#

implementations in the community.

Received: 10 December 2015 Accepted: 12 February 2016 Published: 15 March 2016 set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measureable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that focus on the human scholar, the FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals. This Comment is the first formal publication of the FAIR Principles, and includes the rationale behind them, and some exemplar

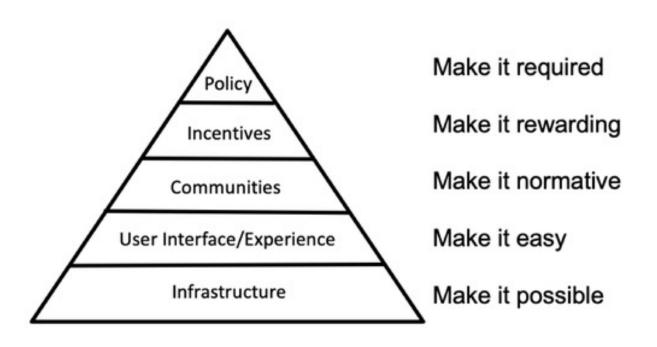
There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse

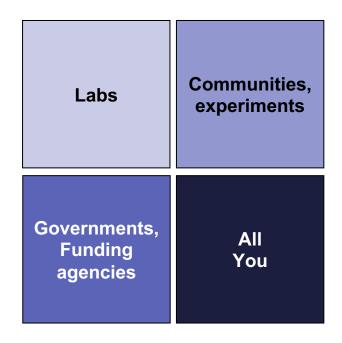
#### FAIR Guiding Principles (2016)

M. D. Wilkinson et al. "The FAIR Guiding Principles for scientific data management and stewardship." *Scientific data* 3.1 (2016): 1-9.

#### What to do?

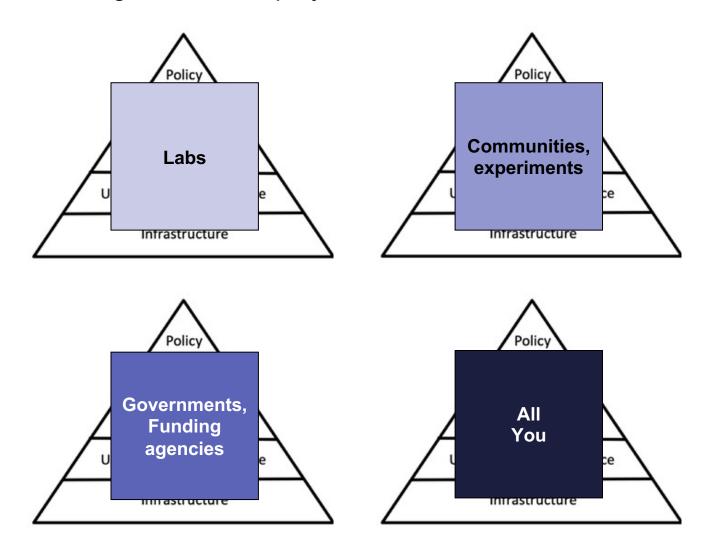
The pyramid of cultural change – different players involved





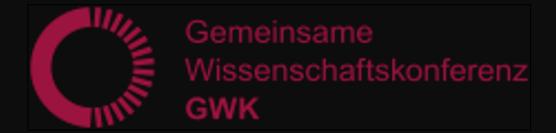
#### What to do?

The pyramid of cultural change – different players involved



# NFDI & PUNCH4NFDI

# Helmholtz Metadata Collaboration HMC



Funded by



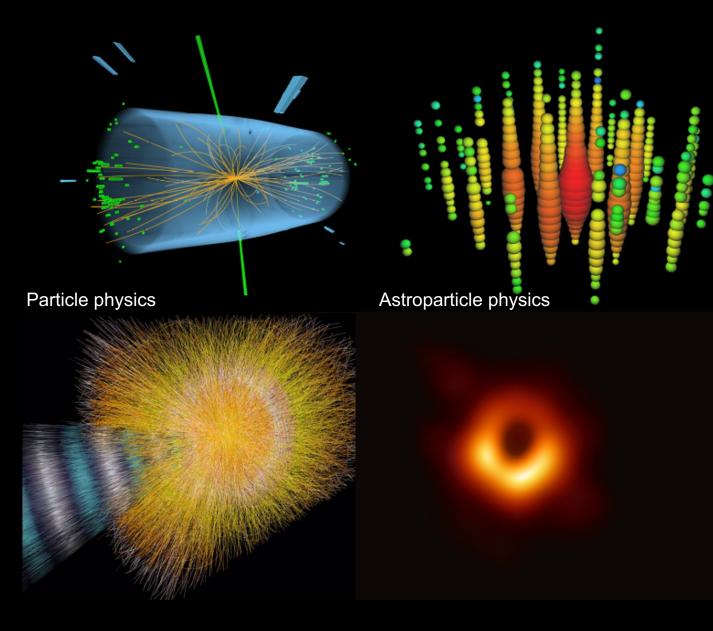
Deutsche Forschungsgemeinschaft

German Research Foundation

# Nationale Research Data Infrastructure (NFDI)

- Sustainable utilisation of research data
- Establishment of FAIR RDM
- Connection to Europe & the world
- Bottom-up approach: 27 consortia
- Base service initiative
- 5 (+5) year funding (PUNCH4NFDI: 3,5MEUR/a)

See also DFG.de/nfdi and nfdi.de



Astronomy

Hadron & nuclear physics



# Particles, Universe, NuClei and Hadrons for the NFDI

The prime goal of PUNCH4NFDI is the setup of a federated and "FAIR" science data platform, offering the infrastructures and interfaces necessary for the access to and (re)use of (meta)data and computing resources of the involved communities and beyond.

#### **NFDI Consortia**



**SSH**OpenCluster



#### Base4NFDI – a Base Service Initiative Across Consortia





WHY B4N

SUBMISSIONS

**HOW B4N WILL DECIDE** 

WHO CAN APPLY AND HOW

**FURTHER INFO** 

- Framework for user-driven basic service development
- Starting with IAM, PID services, terminology services
- Building on existing solutions and complementing EOSC

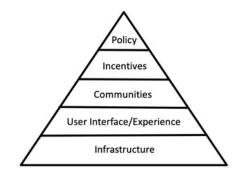
# **Basic Services for NFDI**

Create NFDI-wide basic services in a world of specific domains

# Helmholtz Metadata Collaboration < HMC> | HELMHOLTZ METADATA COLLABORATION | C



- Make Helmholtz data **FAIR**
- Provide services for **sustainable** and efficient metadata handling
- Develop, share and consolidate community-expertise in metadata across Helmholtz
- Address all levels of change pyramid





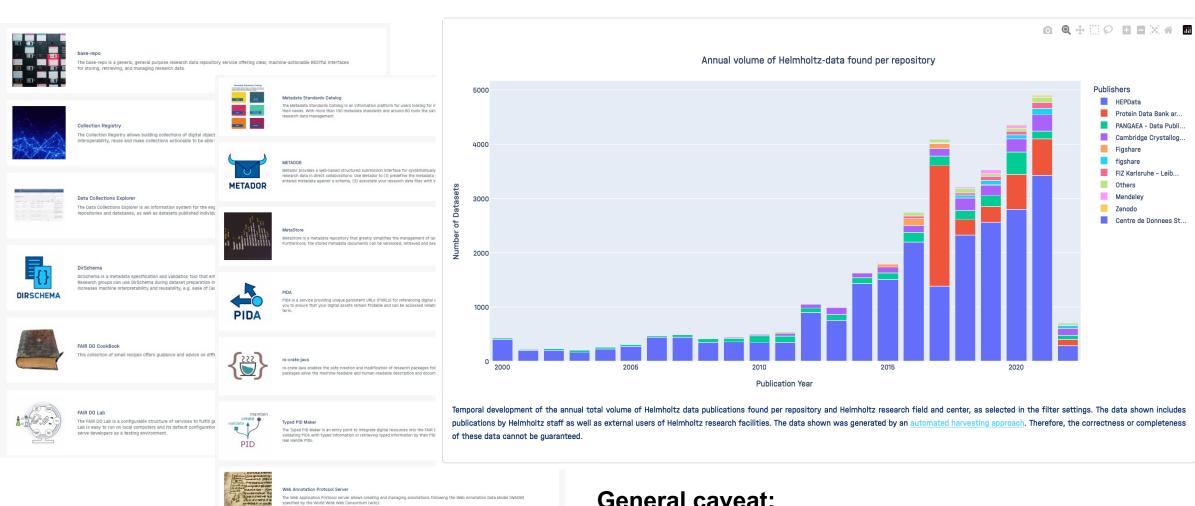
#### **Helmholtz Association: largest** German science organisation

6 research fields, 19 centres, > 40.000 staff, ~ 4.5 billion Euro

# Helmholtz Metadata Collaboration < HMC> | HELMHOLTZ METADATA COLLABORATION | METADATA COLLABORAT



https://helmholtz-metadaten.de/en



#### **General caveat:**

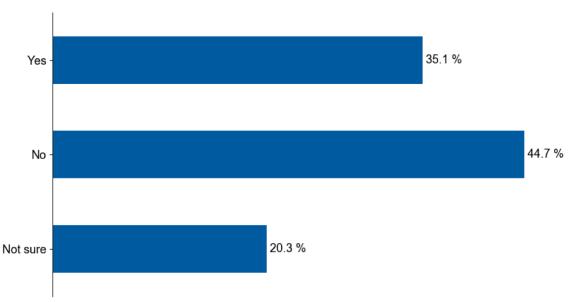
High # of data sets: Harvesting of HEPData

- → usefulness of FAIR indicators / KPIs?
- → What is a useful metric for data sets & software?

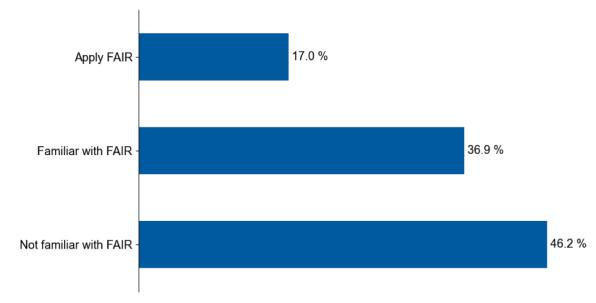
### **HMC Survey**



https://oceanrep.geomar.de/id/eprint/57494/



**Figure 14: "Do you document your research data in a structured way?** (e.g., using forms, templates or schemas)". (Single choice question, available to all respondents, number of respondents who answered this question: n = 582, relative amounts refer to n)

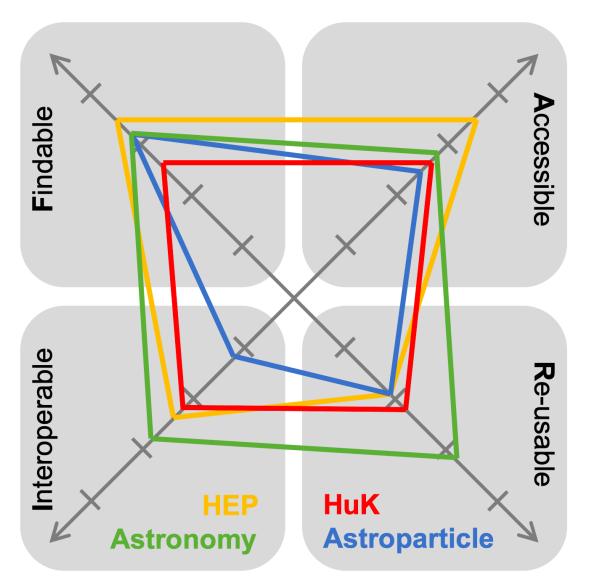


**Figure 8: "How familiar are you with the FAIR data guidelines?".** Question not available to respondents who previously assigned themselves to the Helmholtz research field Information. (Single-choice question, number of respondents who answered this question: n = 559, relative amounts refer to n)

# FAIR Assessment

# Making Things Operational: PUNCH4NFDI Proposal (2020)



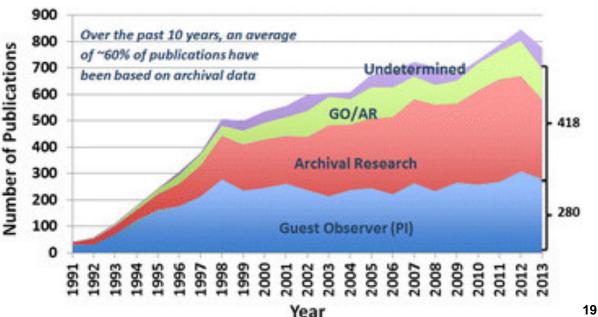


A lot of HEP data are in HEPData (open, F&A), and WITHIN collaborations (e.g. at LHC) data are FAIR. No (?) solutions for medium and small experiments. Limited I&R.

50% of all astronomy publications are based on the re-use of "old" data, and astro data are often open.

There are no attached compute resources.

#### DOI:10.1186/s40192-014-0022-8



## Making Things Operational: FAIR Indicators



# FAIR Data Maturity Model Specification and Guidelines 2020



Proposed RDA Recommendation
Produced by: FAIR Data Maturity Model WG, 2019-2020

https://www.rd-alliance.org/groups/fair-data-maturity-model-wg

https://zenodo.org/record/3909563

#### From 15 FAIR Guidelines (2016) to 41 FAIR Indicators (2020)

1 2 3	<ul> <li>not applicable</li> <li>not being considered this yet</li> <li>under consideration or in planning phase</li> <li>in implementation phase</li> <li>fully implemented</li> </ul>	0 Score 0 0 0 1	
RDA-F1-01M Metadata identified by a persistent identifier ••• Essential			
Principle to which the indicator relates	This indicator is linked to the following principle: F1 (meta)data are assigned a globally unique and eternally persistent identifier.		
Description of the indicator RDA1- F1-01M	This indicator evaluates whether or not the metadata is identified by a <u>persistent</u> <u>identifier</u> . A persistent identifier ensures that the metadata will remain findable over time and reduces the risk of broken links.		
Assessment details	The persistence of an identifier is determined by the commitment of the organisation that assigns and manages the identifier, so the evaluation of this indicator needs to take into account the persistence policy of that organisation. Such a commitment could be expressed by a university or research institute, by a research infrastructure or by an organisation that issues formal identifiers, such as the International DOI Foundation. A possible way to evaluate this indicator is to verify that the identifier used for the metadata is listed in a registry service like the RDA-endorsed FAIRsharing. <sup>15</sup>		

There are ways to measure FAIRness. Details are extremely controversial (scoring systems).

# **Example: EMIL at BESSY (PaN Science)**



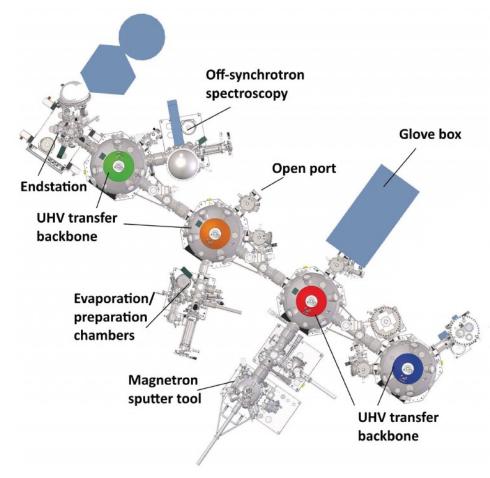


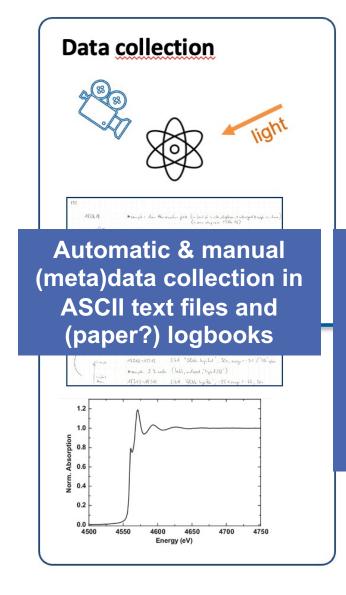
Figure 1: Schematic presentation of the SISSY@EMIL's setup connecting various processing and analysis chambers, among them the SISSY I endstation.

#### Particularly nice example:

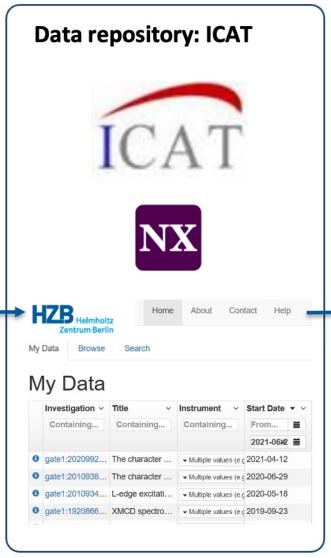
- Integrating entire data collection and processes into FAIR assessment
- Breaking FAIR down to concrete things that can be implemented at the lab level

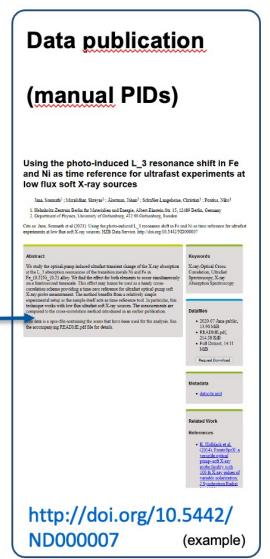
ICALEPS2021, doi:10.18429/JACoW-ICALEPS2021-WEBL05

# **Example from HMC: EMIL at BESSY (PaN Science)**









#### **FAIR Assessment**



#### **Findability:**

- Discovery metadata
- Automatic assignment of PIDs
- Connection to higher-level services









- (meta)data in ICAT repository
- Authentication / authorization





#### Interoperability:

- NeXus format
- ICAT schema (mappings w.i.p.)



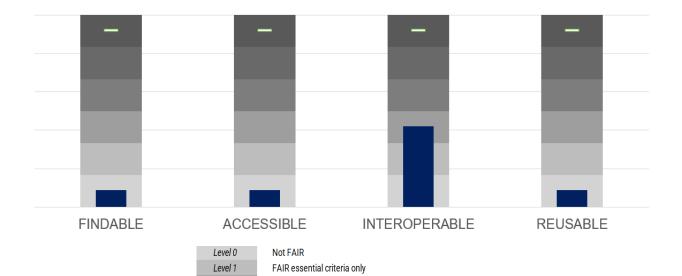


#### **Reusability:**

- Sample + calibration (meta)data
- License metadata







FAIR essential criteria + 50 % of important criteria

FAIR essential criteria + 100% of important criteria

FAIR essential criteria + 100% of important criteria + 50% of useful criteria

FAIR essential criteria + 100% of important criteria + 100% of useful criteria

Level 2

Level 4

Level 5

Numerous approaches; importance of process evaluation. E.g. ...



ICALEPS2021, doi:10.18429/JACoW-ICALEPS2021-WEBL05

# Some Usecases

## The EAJADE Project

Europe-America-Japan Accelerator Development and Exchange Programme A Marie Sklodowska-Curie Research and Innovation Staff Exchange (SE) action, funded by the EU under Horizon-Europe.



















**BERKELEY LAE** 

















Work package title

R&D&I at currently operating state-of-the-art facilities

State-of-the-art high-gradient, high-efficiency, reduced-cost radio-frequency structures and power sources

Special technologies, devices and systems performance

Sustainable technologies scientific facilities

Investigation of potential early of novel applications and advanced technologies for colliders

Management, dissemination. training, knowledge transfer, and communication

# The EAJADE Project



Europe-America-Japan Accelerator Development and Exchange Programme A Marie Sklodowska-Curie Research and Innovation Staff Exchange (SE) action, funded by the EU under Horizon-Europe.

#### **Questions:**

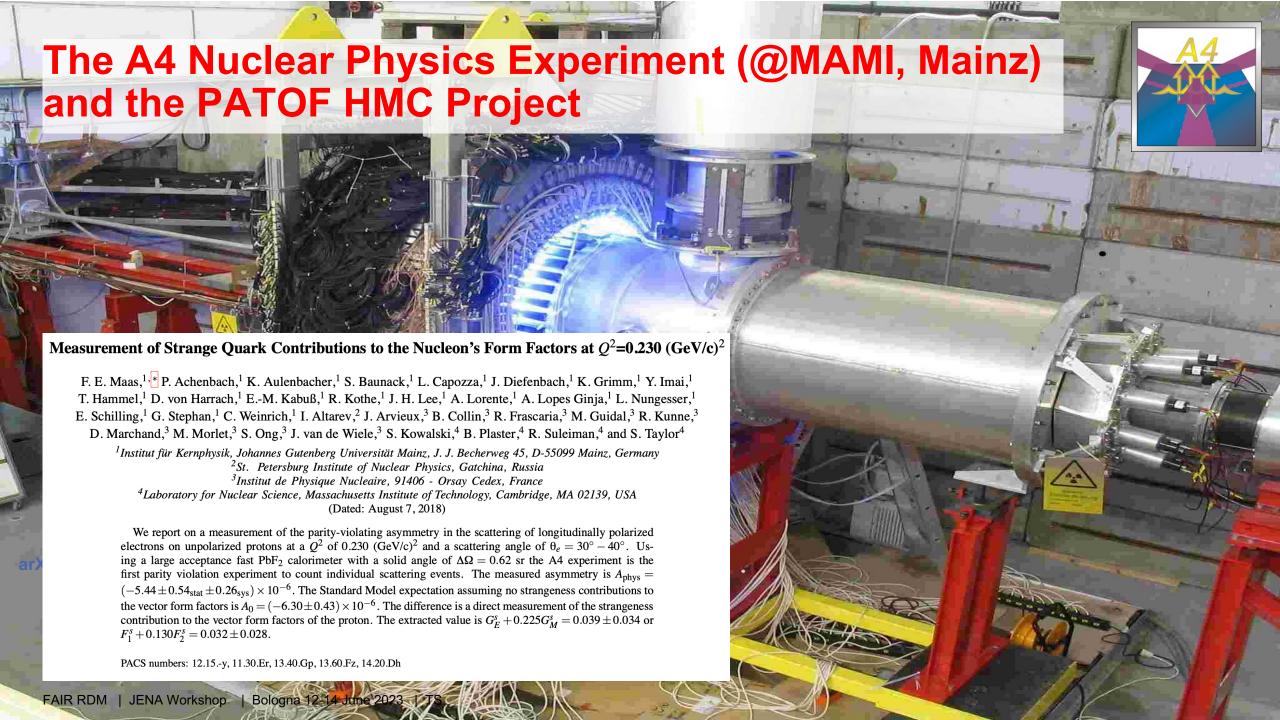
- Where and how do we store what?
- How long do we store? Just the good-practice 10 years? Persistently? What IDs do we give?
- How do we organise access to the data?
- How to create (which) metadata schema and uniform metadata for the project data?
- Who does it? Do we really have to do it? Is it worth it? ...

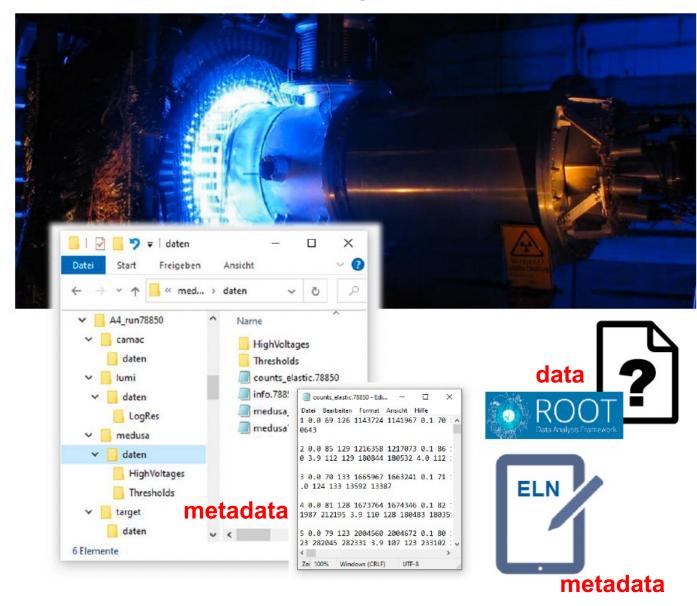
#### Findings:

- There is no clear picture of the data and their future treatment.
- There is no well-specified storage location at hand.
- There is no idea about a metadata schema for this research.
- There is no consensus on the necessity.
- Many technicalities (embargo, AAI, licenses, ..) are absolutely unsolved.
- •



... but working on a (preliminary) solution.





#### A4 Experiment:

- Instrument @ Mainz Microtron
- Already dismounted
- Published papers but potential for more

#### **Prototypical HEP Files:**

- Nested folder structure (unknown context)
- Root Files: community-specific standard
- ASCII Files: Unformatted, minimum metadata
- Electronic Lab Notebook: context (xml)

#### Practical Goal:

- Reusable data from a dismounted experiment
- Template for future instruments

G. Günther

# A4

#### **Assessment**

- ROOT files with customized classes: self-describing, binary, requires full software suite
  - → requires installation of customised classes; version control requires containerisation
  - → solution soon at hand

- © RDA-I1-01D: Data uses representation in standardised format
- © RDA-R1.3-01D: Data complies with a community standard
- ⊗ RDA-I1-02D: Data uses machine-understandable knowledge representation
- ⊗ RDA-R1.3-01D: Data is in machine-understandable community standard
- ASCII files: neither human nor machine readable
  - → require conversion to human / machine-readable XML format, adding metadata through json files (column headers, units, ..)

    RDF appotations provide machine-
  - RDF annotations provide machine-

readable definitions e.g. using ontology QUDT or human-readable context (e.g. using weblinks)

- ⊗ RDA-F2-01M: Rich metadata is provided to allow discovery
- ⊗ RDA-I1-02M: Metadata uses machine-understandable knowledge representation
- ⊗ RDA-R1-01M: Plurality of accurate and relevant attributes allow reuse
- ⊗ RDA-R1.3-02M: Metadata is in machine-understandable community standard

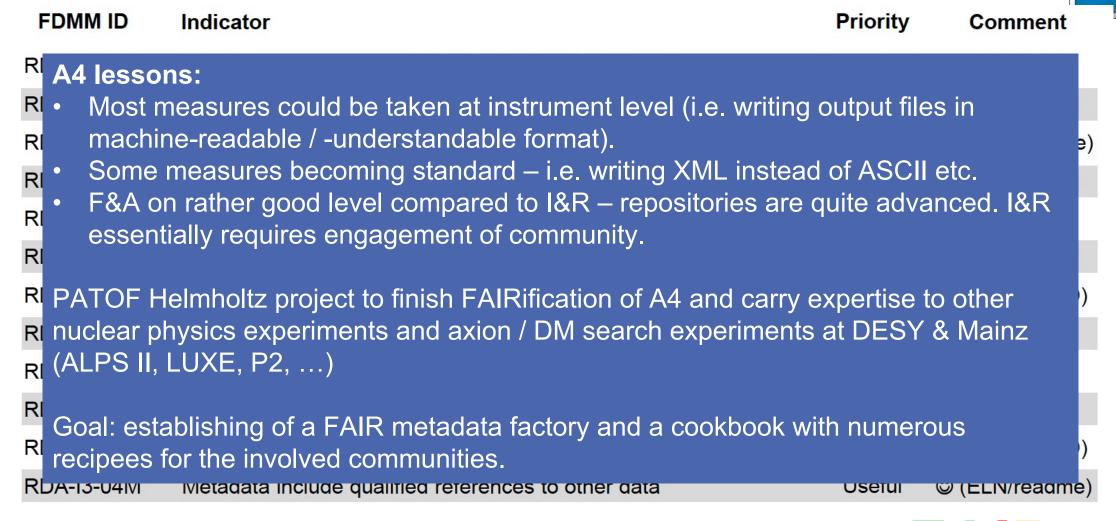
- Electronic lab notebook and readme pages: May contain private / confidential entries
  - → make black/whitelist; transfer to XML/DataCite or html)

- © RDA-I3-01M: Metadata includes references to other metadata
- © RDA-I3-02M: Metadata includes references to other data

G. Günther

FDMM ID	Indicator	Priority	Comment
RDA-I1-01M	Metadata uses representation in standardized format	Important	☺ (DataCite)
RDA-I1-01D	Data uses representation in standardised format	Important	☺ (root/class)
RDA-I1-02M	Metadata uses machine-understandable knowledge representation	Important	
RDA-I1-02D	Data uses machine-understandable knowledge representation	Important	<mark></mark> (root/class)
RDA-I2-01M	Metadata uses FAIR-compliant vocabularies	Important	☺ (DataCite)
RDA-I2-01D	Data uses FAIR-compliant vocabularies	Useful	⊗ (root/class)
RDA-I3-01M	Metadata includes references to other metadata	Important	☺ (e.g. ORCID)
RDA-I3-01D	Data includes references to other data	Useful	(root)
RDA-I3-02M	Metadata includes references to other data	Useful	☺ (via ELN)
RDA-I3-02D	Data includes qualified references to other data	Useful	(root)
RDA-I3-03M	Metadata includes qualified references to other metadata	Important	☺ (e.g. ORCID)
RDA-I3-04M	Metadata include qualified references to other data	Useful	© (ELN/readme)





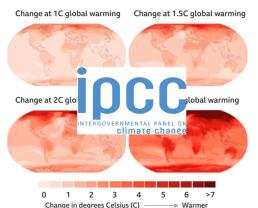


# **Irreversibility Challenge**

# FAIR???

#### Increasing data volumes require more and other metadata

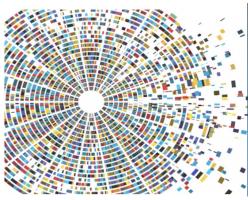
Advancement of knowledge and solutions to societal challenges depend on ICT resources & software. Data increase requires new approaches to scientific computing and data management, changing today's paradigms. This requires long-term R&D plan with coordinated efforts from different communities & large R&D investments.



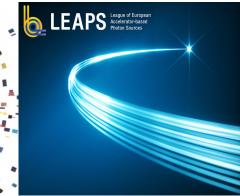
Climate modelling: CMIP6 with 22 PB and 7M data sets



SKAO (> 2027): 600PB/a (archived); MeerKAT (now): 3 PB/d (produced + analysed + cancelled)



Genomics / biomedicine: complex long time series



Light sources: 35k users. TB/s per facility. Factor 10<sup>4</sup>-10<sup>6</sup> data rate increase in this decade



The "smart city" produces massive amounts of data

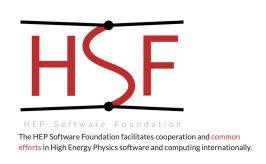
Requires in-flight analytics, data reduction / compression / loss / removal, federated & heterogeneous resources, green IT, ... To tackle **irreversibility challenge and democratise analysis**: Massive investment in metadata annotation and FAIR & open data (1/3 data, 1/3 metadata, 1/3 simulation) -> role of EU funding!

# (Infra)Structures Culture Boundary Conditions

# Make it possible, easy (normative, rewarding)

Technical and conceptual solutions, individual services, single experiences ...

















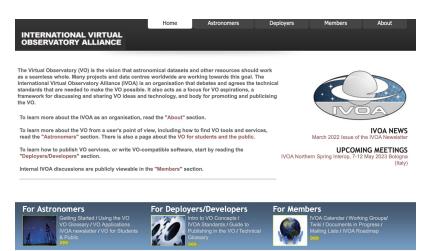






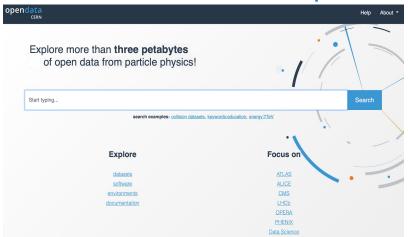
# Make it possible, easy (normative, rewarding)

#### Labs, collaborations, communities, ...



#### **Virtual Observatory**

#### **CERN Open Data**





# **European structures and services German ErUM-Data (erumdatahub.de)**





# We are a Digital Knowledge Agent

The ErUM-Data\_Hub, funded by the Federal Ministry of Education and Research (BMBF), is a central networking and transfer office for the digital transformation in the exploration of universe and matter (German abbreviation: ErUM). The main aims of the ErUm-Data-Hub are: The networking of ErUM-communities, identification and exploitation of synergies in ErUm-Data-projects in the field of digitalization, the communication of research results geared to the target groups as well as knowledge and innovation transfer. Furthermore, the ErUM-Data-Hub provides a diversified further education offer in the field of digital competence.

As part of the **ErUM-Data Plan of Action**, the ErUM Data Hub pursues the overarching goal of digital transformation in fundamental ErUM-Pro research. Read more about who we are and what we do.



MEETINGS PANELS STATEMENTS LINEAR COLLIDER ACTIVITIES



International Committee for Future Accelerators

#### **ZENODO**



# Make it normative (possible, easy): Policies

#### All Helmholtz centers should have a data policy in place

According to the position paper on the handling of research data in the Helmholtz Association (Mitgliederversammlung der Helmholtz-Gemeinschaft, 2016), all member centers are expected to have a policy in place by the end of 2017. "All member Centres need to have established guidelines by the end of 2017. Formulation of the discipline-specific details is expected to take some years."

Helmholtz Open Science Policy (2022) also emphases having publicly available policies for all the Helmholtz Centers: "All Centers will establish detailed procedures for managing research data in publicly available policies, and will regularly examine and if necessary adapt these procedures."

Digital research data generated should be managed in accordance with the FAIR principles

According to the new Helmholtz Open Science Policy (2022), the employees shall ensure that the digital research data that they generate shall be managed responsibly and in accordance with the **FAIR Principles**.

Retention of research data should be guaranteed for 10 years

DFG Guidelines for Safeguarding Good Research Practice (2022) says that "When scientific and academic findings are made publicly available, the research data (generally raw data) on which they are based are generally archived in an accessible and identifiable manner for a period of **ten years** at the institution where the data were produced or in cross-location repositories".

- FAs and institutions must issue RDM policies – creating pressure in two directions: users must comply, institutions must make it possible (funding).
- Example: Helmholtz now preparing for including FAIRness of produced data sets in its KPIs for the next funding period.

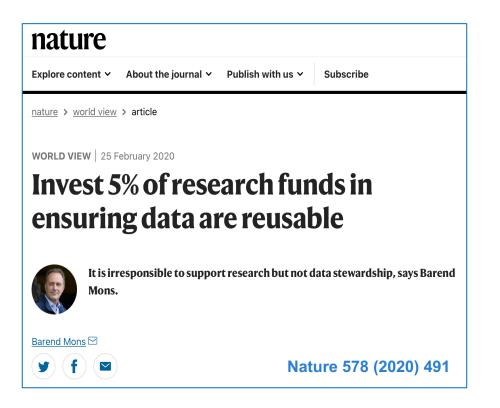
Helmholtz Open Science policy https://gfzpublic.gfz-potsdam.de/rest/items/item\_5013535\_1/component/file\_5013536/content

# **Funding Agency Level**

Policies, requirements, funding, ...

EU, German Research Association DFG (and certainly others) (need to)issue policies, and they require us to provide FAIR, sustainable and open data management.

But (today mostly) no dedicated funding for data management, data curation in projects.





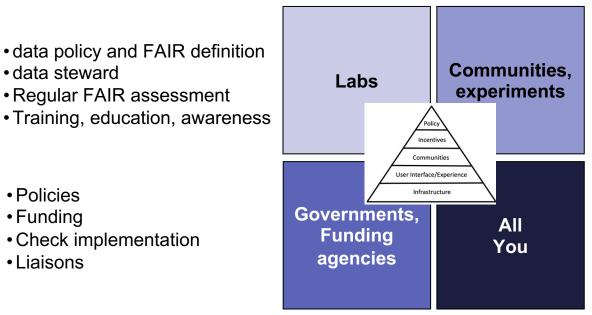


# Conclusions

# **The Large Picture - Requirements**



- data steward
- Regular FAIR assessment
- Training, education, awareness
- Policies
- Funding
- Check implementation
- Liaisons



- Funding applications
- Standards and terminologies
- Recognition
- Communication
- Global AAI
- Change of mind
- Think metadata (1/3,1/3,1/3!)

- Challenges require massive metadata harvesting – with tools that are not yet there.
- ML → need to harvest as many as possible machine-actionable metadata!
- Necessity of long-term investment plan!

#### **Essential Tools for FAIR PUNCH Data**





**Digital** research products



Workflows **Algorithms** 













**FAIR** 



**Software** 



Metadata (schemas)

1/3 data 1/3 metadata 1/3 simulation



Money



**Policy** 



**Data stewards** 



**Assessment** 



**Training Education** Communication



**Awareness** 

# On Open Data

#### I Can't Publish My Data! Lame Excuses and Some Answers

Markus Demleitner

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#### Abstract

You already know why publishing data is the right thing to do, don't you? It's just that exactly your data is an exception, right? It cannot be published because...

Here's a collection of reasons we've heard. And some replies we've always wanted to give (but mostly swallowed).

#### Acknowledgement

reward you plenty.

The good parts of this were blatantly snarfed from Charly Strasser's brilliant web page http://datapub.cdlib.org/ closed-data-excuses-excuses/

My data is too complicated

Be that as it may: Try explaining anyway,

the improved understanding you'll get will

sure you've understood it yourself?

If it's too complicated to explain: are you

#### People will misinterpret my data

Good documentation and standards mitigate this.

As for what remains - well, if you're publishing prose (i.e., in a journal), how many of your readers do you think actually get what you're writing?

#### I might yet want to use it

... in the great seminal research paper I've always wanted to write.

If you've not done so so far, will you at all? When? Too much data obtained for uncounted kilodollars (or megadollars, for that matter) is gathering dust, waiting for the "real soon now". Be fair to the world and to the people funding you and your research and publish the data. If you're really worried, put a one-year embargo on the material.

Procraste's Law: If over a year you don't get to do it, chances are overwhelming you'll never do it.

My data is boring

Leave that decision to others. You'd be

surprised how much "boring data" people

tables in the sweat of their mice. Every

#### I'm busy

... and it's not a priority.

A-ha! Here we're talking. True, the current system of rewards in science doesn't actually encourage data publishing. But publishing is the right thing to do, anyway, even before the system gets back on a path of recovery. And: more and more funding agencies at least sound requirements for data publishing and preservapoint-and-click out of printed graphs or tion.

It's too much work

No. it's not. For example, the GAVO

data center is there to help you. Unless

you data is particularly funky, you'll not

have to spend more than half a day from

the half-documented, messy goo that's on

your disk to a shiny, blinking, proper, VO-

registred, be-proud-of data service. And we'll take care of it henceforth.

#### I'm not sure I own the data

That's amazingly common. So: Are you sure you cannot find out who does? If you made a reasonable effort to figure that out but failed, the likelihood is high you've orphaned data on your hands, obtained by people who've long left science for greener

To avoid similar uncertainties with your data later on, please consider assigning explicit licenses to it - ideally CC-0. Do not worry that people will not give credit just because of a Free license. We're in science, and so this is a matter of scientific conduct rather than the law.

... or at least not very interesting.

#### People will contact me

how much you learned by asking other people.

Plus, you'll notice that quite a few of those questions are actually quite clever, so answering them is a good use of your

As to the stupid questions - well, they are annoying, but at least for us even those were eye-openers now and then.

and ask about stuff.

Well, science is about exchange. Think

Ask around at the booth for more infor-

# http://docs.g-vo.org/talks/2013-tuebingen-lameex.pdf

(Markus Demleitner)

#### My data is embarrassingly bad

Everyone's is. Good data is just bad data that more eyes have seen and more hands have improved.

# Thank you!

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# Acknowledgements







