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A Metadata Model for Harmonising Engineering Research Data Across Process and Laboratory Boundaries

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Presenter: Dipl. – Ing. Felix Conrad

Professional Experience

July 2019 Diploma degree, Mechanical Engineering
August 2020 Doctoral Researcher, TU Dresden, Germany

Publications

- Benchmarking AutoML in materials design npj scientific reports
- AutoML Applied in Production Engineering Proc. Comp. Science
- Need for UAI – Anatomy of Usable Artificial Intelligence MDPI MTI
- Comparative Analysis of Small Data Acquisition Strategies IARIA Software
- Impact of Data Sampling on Performance of ML-Models WGP 2022

Research Interest

- Machine-learning for Materials Design
- Automated Machine-learning
- Usable AI



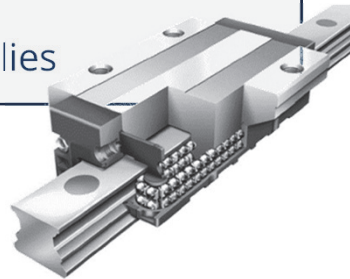
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TUD Dresden University of Technology
Institute of Mechatronic Engineering
Department Machine data utilisation

TUD - Department "Machine data utilisation"

Using data for production technology

Machine health

- Failure detection
- Prediction of anomalies



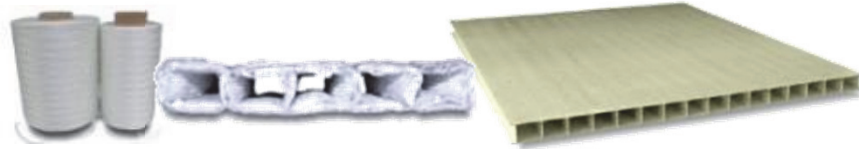
Machine operation/start-up

- Process/station monitoring
- Monitoring operating accuracy



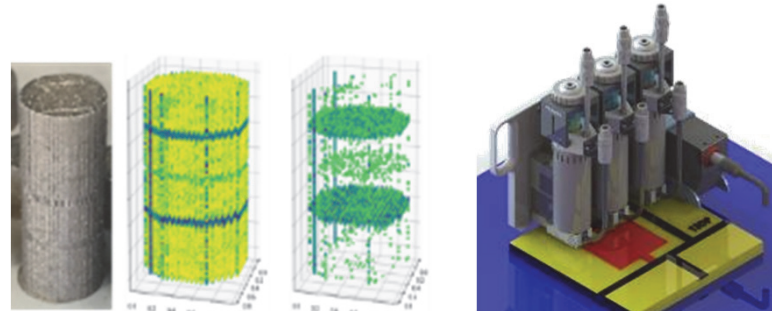
Manufacturing process chains

- Exploring effects
- Overarching correlations



Quality and process

- Quality prediction
- Finding optimal process parameters



Method development

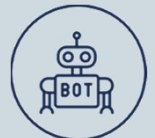
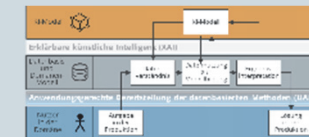
AI algorithm selection and testing



Abstraction in workflow models



User-friendly provision - UAI



Research data management



Content

Motivation

Use case GRK (Research training group) 2250

- Introduction of GRK 2250
- Status of the Research Data Management

Useable FAIR - Solution approaches for Research Data Management

- Thesaurus for Metadata
- Process data model

Results

Conclusion and outlook

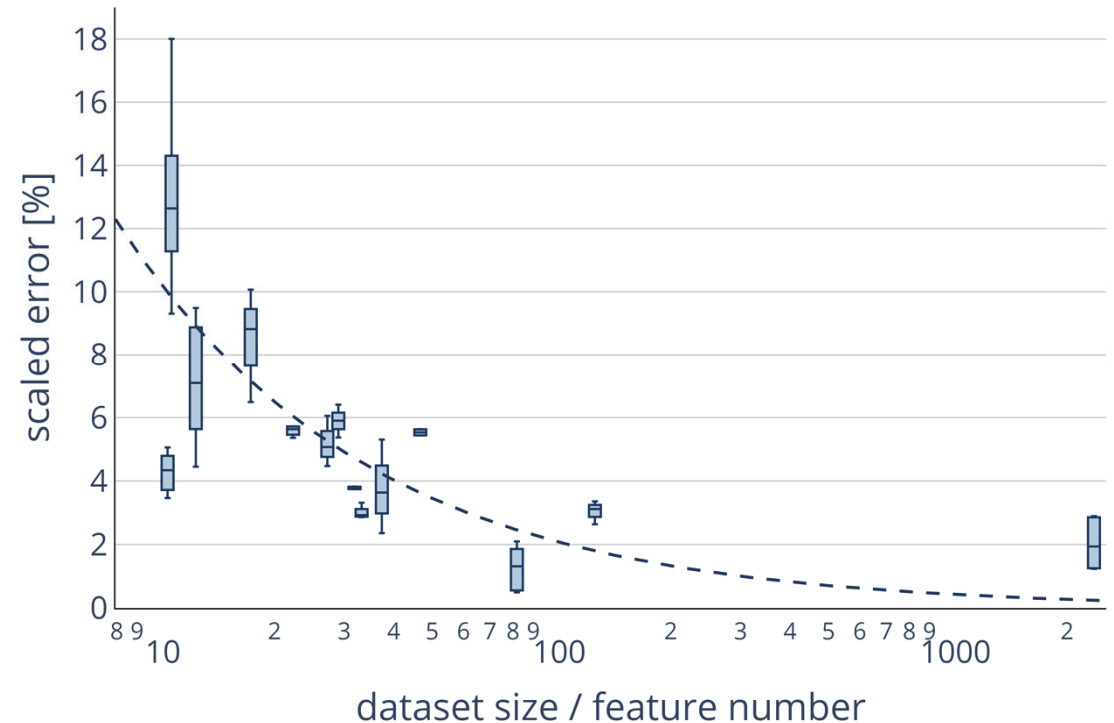
Motivation

Research Data Management perspective

- Fulfilment of the FAIR principles
- Sustainable data management
→ Ensure reusability of data
- Costly experiments in terms of time and resources
 - Drop-Tower-Experiment:
 - Costs for 1 test: ~ € 2,000
 - preparation time: 7 months

Machine learning perspective

- More data leads to better models
- 12 datasets from materials design domain:

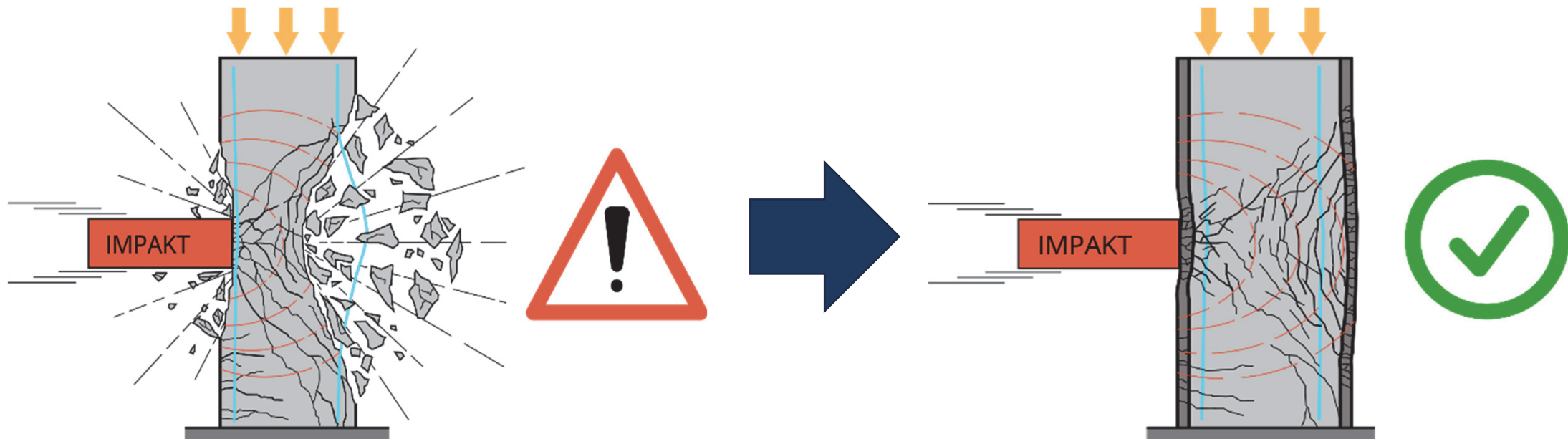


Wiemer, H.; Conrad, F.; et al.: *Illustration of the usable AI paradigm [...] (2023)*

Project GRK 2250: Mineral-bonded composites for enhanced structural impact safety

Overall objective of GRK (Research training group) 2250:

- New generation of textile reinforced mineral-bonded composites
- Theoretical, numerical and data-driven modelling
- Application for the reinforcement of existing structures



graphic: **Curosu et al. (2019)**,
DOI: 10.21012/FC10.235408

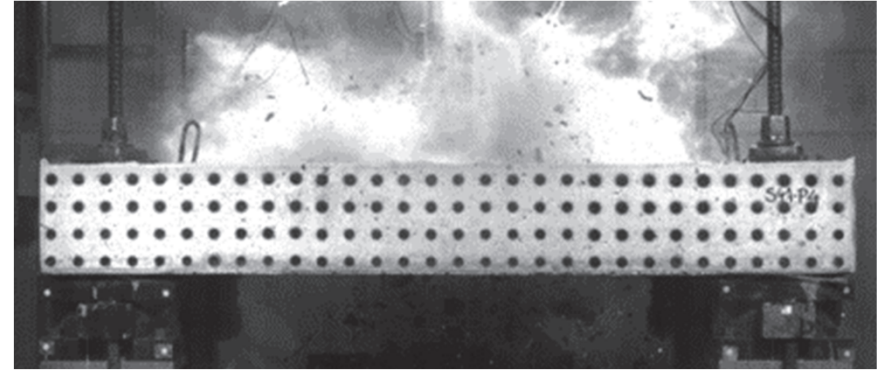
More information: <https://www.grk2250.de/>

Project GRK 2250: Mineral-bonded composites for enhanced structural impact safety

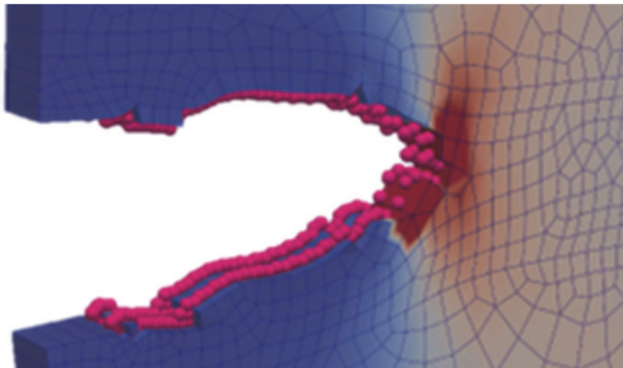
Experimental: material development



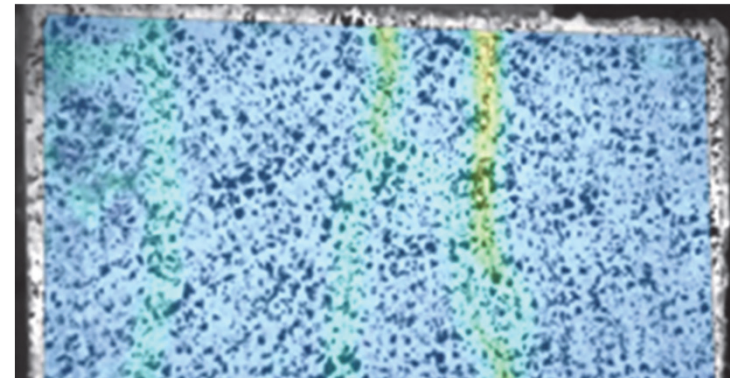
Experimental: structural assessment



Numerical simulation



Data driven and cross-disciplinary



Status quo: Research Data Management in GRK 2250

What:

- Three periods with changing researchers, totalling ~40 researchers over 9 years
- Cumulative data volume of 10 terabytes from ~15 test systems across six laboratories
- Each test system conducted 20 to 300 experiments

How:

- Infrastructure:
 - Shared drive accessible to all partners
 - Mostly Excel spreadsheets or .csv files for (meta)data storage
- Highly manual workflow

Result:

- Unstructured storage of research (meta)data

Approach: FAIR – extension to Useable FAIR



Findable

- Unique identifiers
- Rich metadata
- (Meta)data in a searchable resource



Interoperable

- Meta(data) using common standards + vocabularies
- Integration with other meta(data) enabled.



Usable

The data management system:

- Easily adapted by data curators to research network
- users can store, edit and use (meta-)data that complies with FAIR with minimal effort.



Accessible

- open access
- long-term accessibility

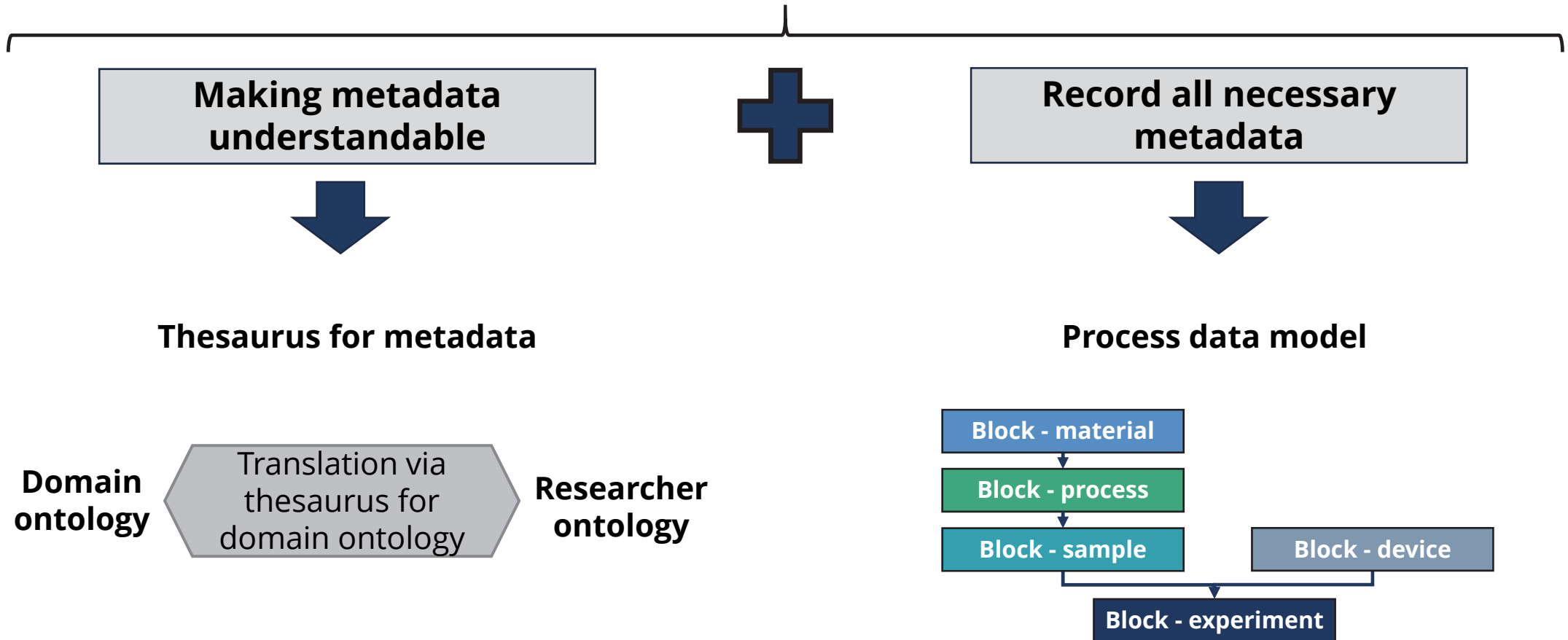


Reusable

- Meta(data) is prepared for easy reuse, with domain-relevant community standards

Approach: FAIR – extension to Useable FAIR

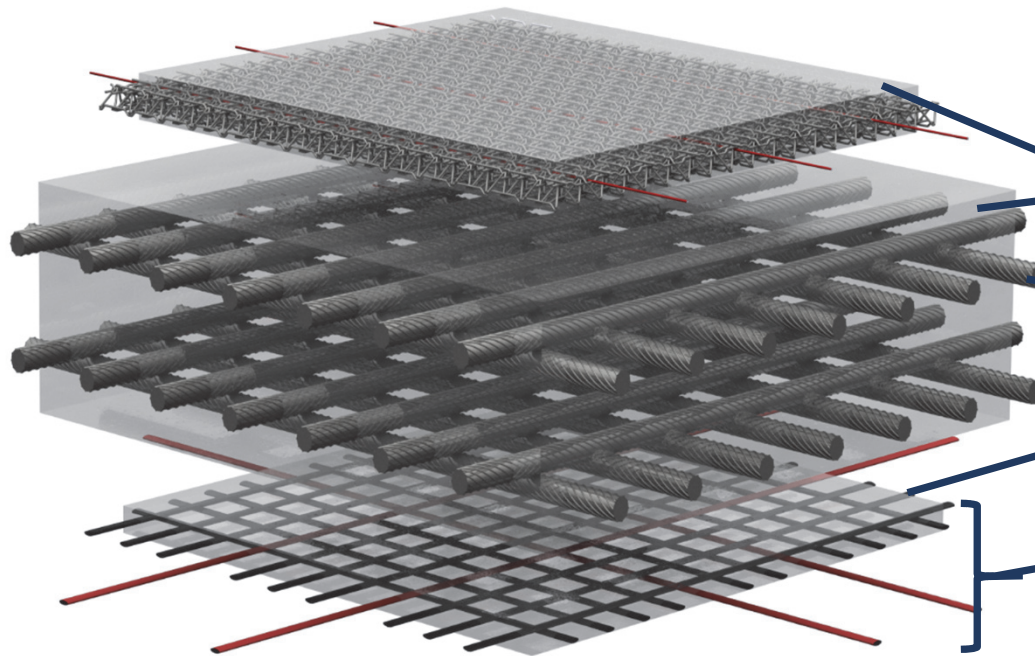
Requirements for cross-process research data management



Approach - 1 : Problem - Diverse Standards in Materials Testing

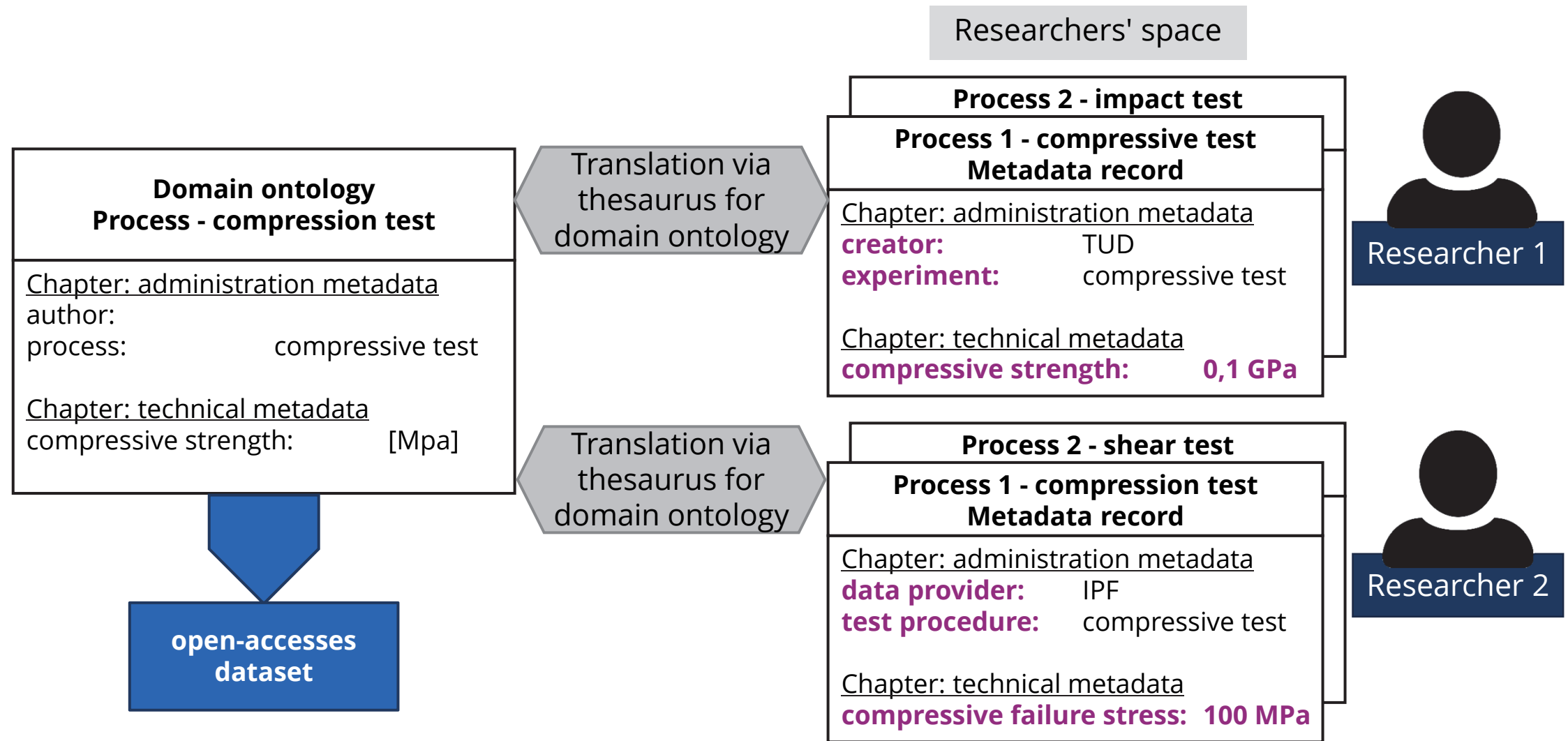
Different conventions in international standards for the same physical properties

- **Example compression test:**



Standard	Material	Symbols	Naming
ISO 1920-4	Concrete	f_c	compressive strength
DIN 50106	Metals	R_{dB}	compressive strength
ISO 604	Plastic	σ_m	compressive strength
ISO 14126	Fibre-reinforced plastic	σ_{cM}	compressive failure stress

Approach - 1 : Problem - Diverse Standards in Materials Testing



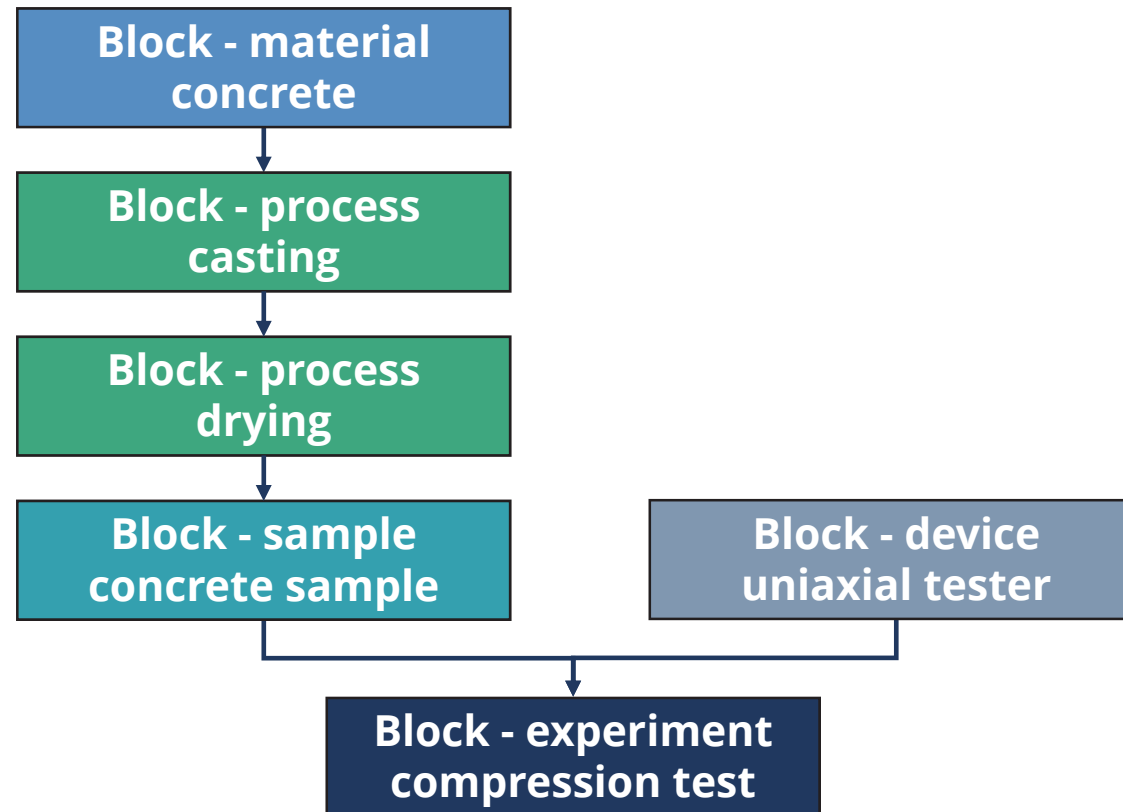
Approach - 2 : Process Data Model

Problem:

- Processes can only be stored reproducibly if the entire process chain is stored reproducibly

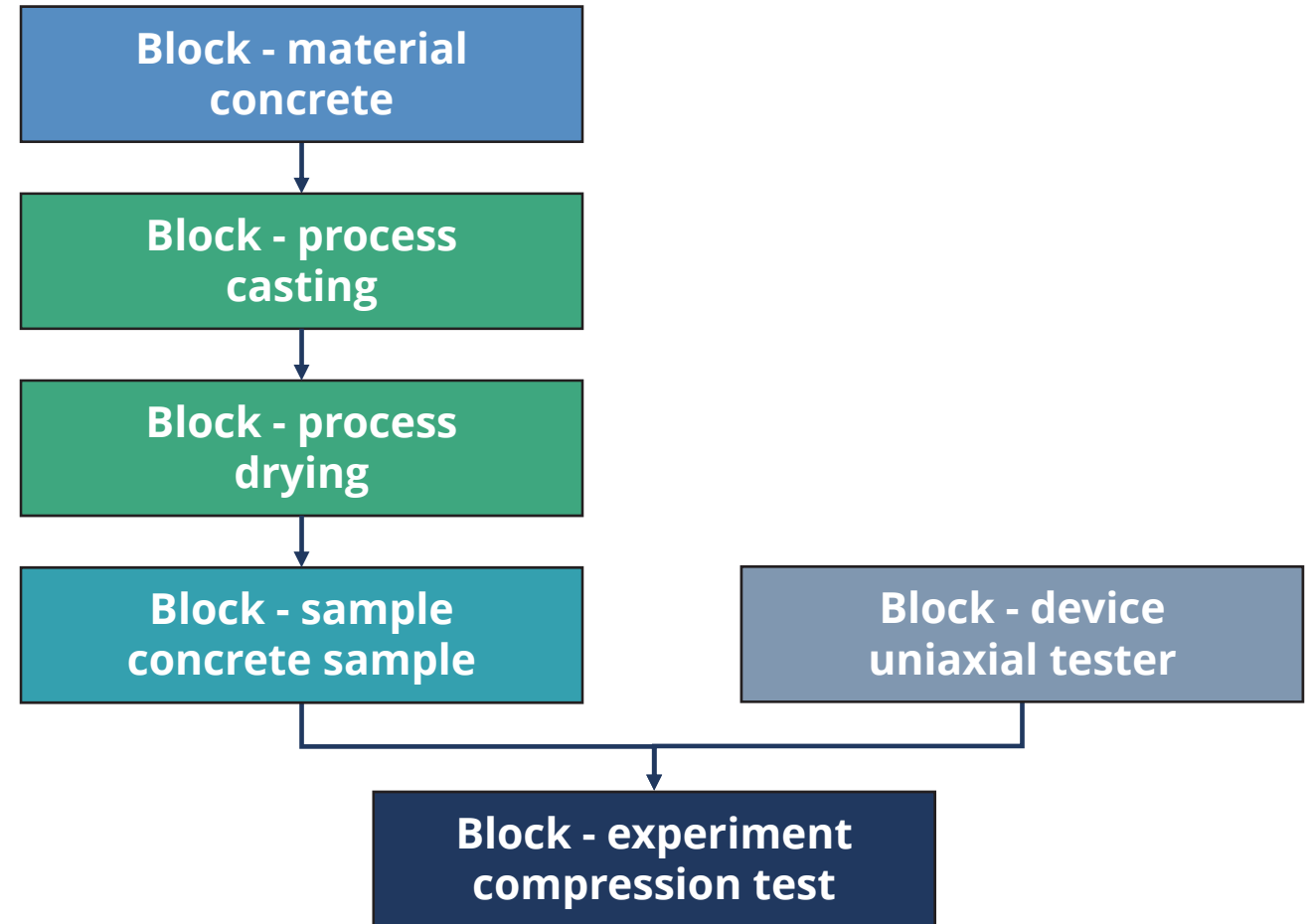
Solution:

- Process Data Model*



Approach - 2 : Process Data Model

Block - material concrete	
<u>Chapter: administration metadata</u>	
author subproject	"Felix Conrad" "C3II"
<u>Chapter: technical metadata</u>	
water content	150 kg/m ³



Approach - 2 : Process Data Model

Metadata library	
subproject	
datatype choice	string ["A1I";...;"C3III"]
compressive strength	
datatype unit	float [MPa; GPa]
⋮	

Block library

Block - material
concrete

Block - process
casting

Block - process
drying

Block - sample
concrete sample

Block - device
uniaxial tester

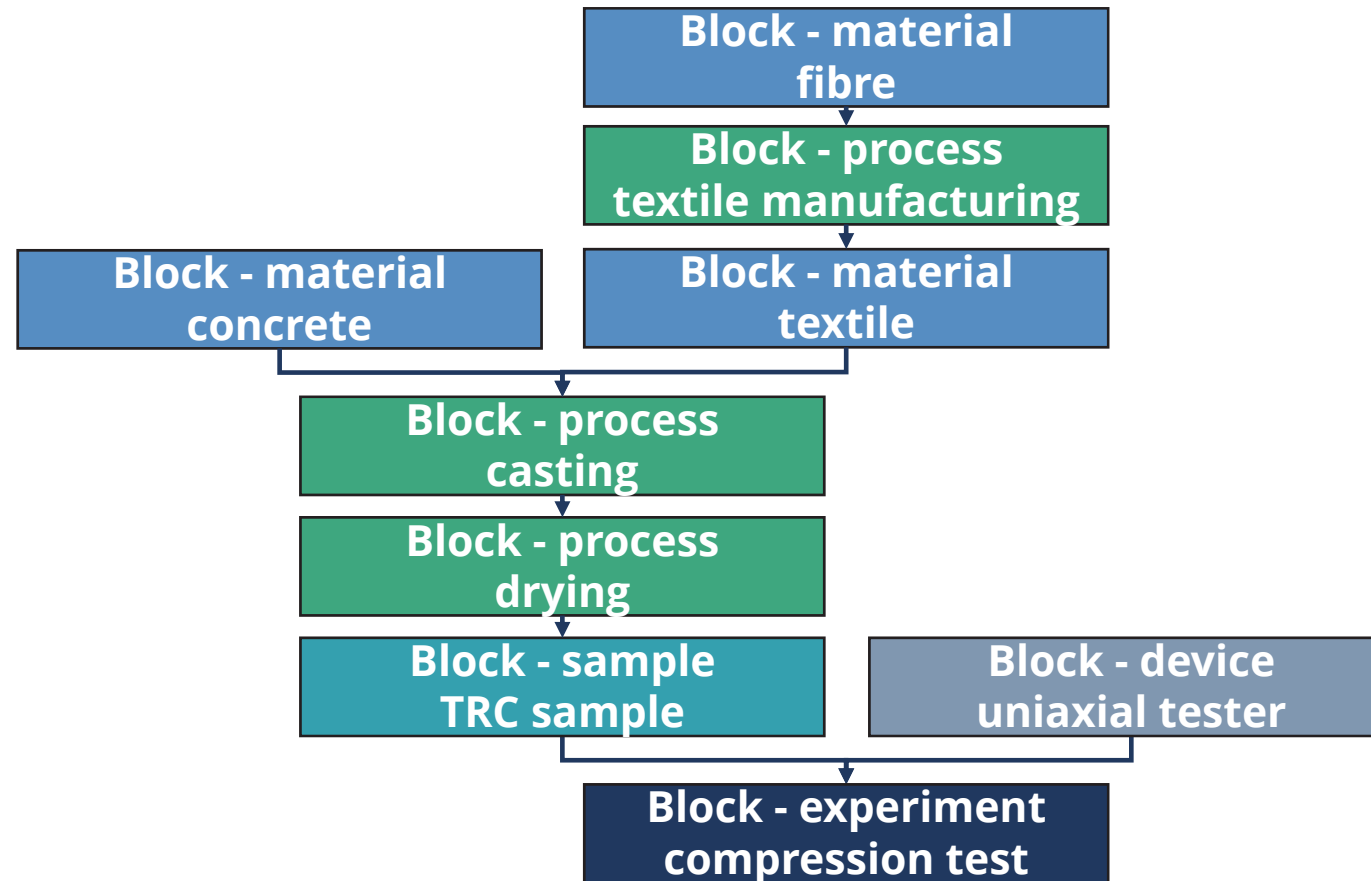
Block - experiment
compression test

Block - experiment compression test	
<u>Chapter: administration metadata</u>	
author subproject	"Felix Conrad" "C3II"
<u>Chapter: technical metadata</u>	
compressive strength	100 Mpa

Approach - 2 : Process Data Model

Process data models crucial for long and branched process chains

- **Example:** Compression test of textile reinforced concrete



Results: Example of a Combined Dataset

Combined Dataset: different processes provided by different institutions:

- Experiment 1: compressive test of textile reinforced concrete – Institute 1
- Experiment 2: compressive test of plain concrete – Institute 1
- Experiment 3: shear test of textile reinforced concrete – Institute 2

	Features				Labels		
	composition: textile	composition: matrix	production composite	test settings: compression test	test settings: shear test	compressive strength	shear strength
1	compression test: textile-reinforced concrete					f_c	
2		compression test:		plain concrete		f_c	
3	shear test: textile-reinforced concrete						τ_{max}

Results: Implementation of RDM Platform

Platform ensures FAIR principles :

- Findable
- Accessible
- Interoperable
- Reusable

DETECT DATA OVERVIEW

SELECT SHOW METADATA PARAMETERS

all main empty

show Filters (Showing rows: 37/37)

current selection:
2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/AIII_Fib-QS-Tens/S-1.4301HD-0

CONFIRM DATA AND GO TO ANALYSIS

DOWNLOAD DATA

SPECIFY DIRECTORY

No directory specified. Check complete group drive.

CHECK FOR NEW DATA

OVERVIEW AND ANALYSIS

file data overview group data overview unsorted data sessions

ID	CREATOR	DATE
2 Projects GRK 2250 II/12 C3II_Felix Conrad/C3II_new-data-cache	Conrad, Felix	2023-11-01
2 Projects GRK 2250 II/12 C3II_Felix Conrad/C3II_Data-structure-2-csv	Conrad, Felix	2023-09-20
2 Projects GRK 2250 II/12 C3II_Felix Conrad/C3II_Data-structure-2c	Conrad, Felix	2021-03-11
2 Projects GRK 2250 II/12 C3II_Felix Conrad/C3II_Data-structure-2	Conrad, Felix	2021-03-11
3 Projects GRK 2250 III/12 C3III_Jinghou Bi/C3III_LC3-2S-PET	Ameer H Ahmed	2023-08-16
3 Projects GRK 2250 III/3 A3III_Ameer H Ahmed/C3III_LC3-2S-PET	Ameer H Ahmed	2023-08-16
2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/AIII_Fib-CY-Tens-Res-S-1.4301HD-0.8	Le Xuan, Hung	2021-01-18
2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/AIII_Fib-QS-Tens	Le Xuan, Hung	2019-02-05
2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/AIII_Fib-QS-Tens-Res-WT1-SESMA-0.3	Le Xuan, Hung	2021-04-28
2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/AIII_Fib-QS-Tens-Res-CF-HTA40-07	Le Xuan, Hung	2021-12-09

ID	EXPERIMENT-ID	+GROUP.NAME	DATE	+FILE.PATH	+FILE.DATE	+GROUP.STATUS
2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/AIII_Fib-QS-Tens	190205_S-1.4301HD-0.8	S-1.4301HD-0.8	190205	2 Projects GRK 2250 II/1 AIII_Hung Le Xuan/01_Experiments/01_Fib-QS-Tens_Duy/02_Analysts/190205_S-1.4301HD-0.8/190205_AIII_Fib-QS-Tens_S-1.4301HD-0.8.xlsx	2022-03-30T09:29:27Z	OK



Further tools for researchers:

- Visualisation of Data
- Analysing Data

Conclusion

- Strategy **harmonizes diverse working cultures** of researchers across domains
- Metadata model **allows merging data:**
 - from similar processes provided by different institutions or fields
 - Merging data from different processes along a process chain

Outlook

- **Completion of the implementation** to a full research data management tool
- **Usability** aspect not fully investigated:
 - **Participant engagement** remains to be analysed
 - **Easy transferability** of the implementation to other research projects to be investigated

Thank you for your attention!

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