Program MSE
MSE Day 18.11.2022

The Long and Winding Road:
News from the Metadata Working Group

Richard Thelen, KIT

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Background

- Till 2002: engineer at Siemens Electronic Assembly. Quality engineer for final product tests of PSGA.

- Since 2003: employee at IMT. MST, QM and metrology.

Some jobs:

1. Member of Prof. Hölscher group *Biomimetic Surfaces*
2. Responsible for two surface characterization labs at IMT
3. Technology expert for AFM within KNMF-i
4. PI for *Correlated Characterization* at IMT
5. MDMC member with focus on metrology issues
6. Vice chairman of DIN committee NA027-03-03
7. …

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Outline

➢ Team

➢ Idea

➢ Approach

➢ Processes described

➢ Issues

➢ Conclusion and Outlook

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The Team

As the MDMC Metadata Working Group, we include:

- ERC

- FZJ

- KIT

- Hereon

- CNR-IOM

… and we are open to others!

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The Idea

As a Metadata Working Group, we focus on:

- Ontologies

- Standardization

- FAIR Data

- Experimental workflows

to create the digital twin of real processes
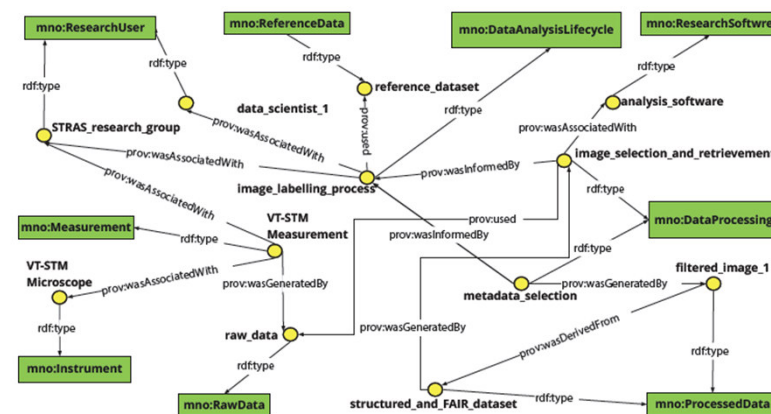
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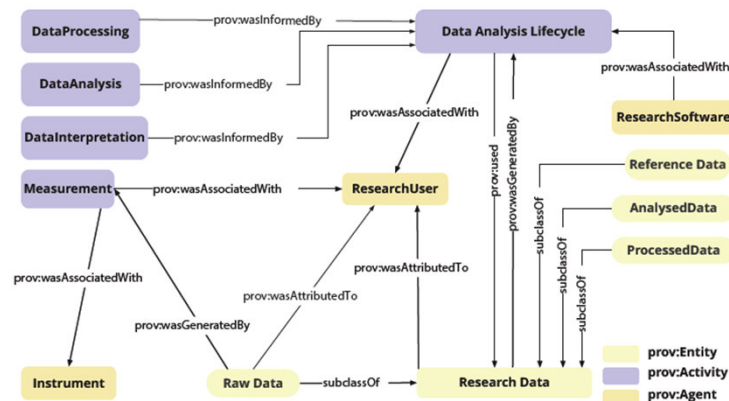
Approach

How to start:

- Define common terminology

- Describe our individual processes

- Generate a model

- Feed it with real (meta)data

- Assess the results

- Draw conclusions

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Approach

Finding the Right Words …

- MDMC-NEP Ontology developed and first application on STM:
  DOI: 10.5445/IR/1000152174

- Cross check with NFFA, NFDI consortia, HMC, RDA, …

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Approach

General Process Knowledge

Input **Process** **Output**

Main Processes
- Manufacturing
- Measuring
- Data Treatment
- Programming
- Administration

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Approach

Structuring present Process Knowledge

Key Issue
Describing generalized processes so that
they fit to individual processes easily

Contradiction !

Granularity used is fine enough to make
individual process description straightforward

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Approach

Processes described

- At KIT: IMT, mainly metrology processes, now general manufacturing processes

  INT, mainly FIB, SEM and TEM

- At FZJ: Ontology development

- At Hereon: Cast based and powder based material development

- At CNR-IOM: FAIRification of STM process
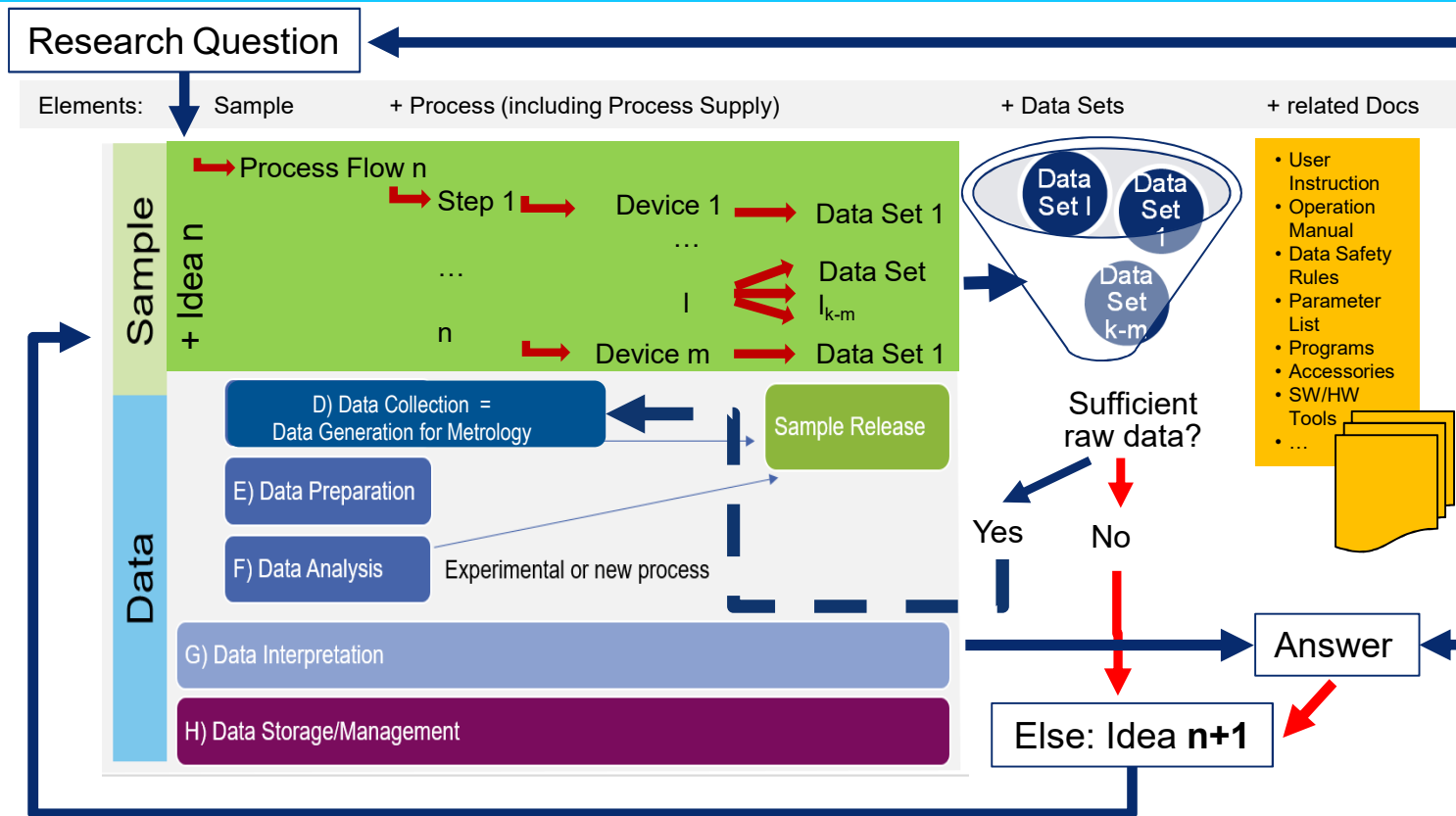
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KIT Metrology Process

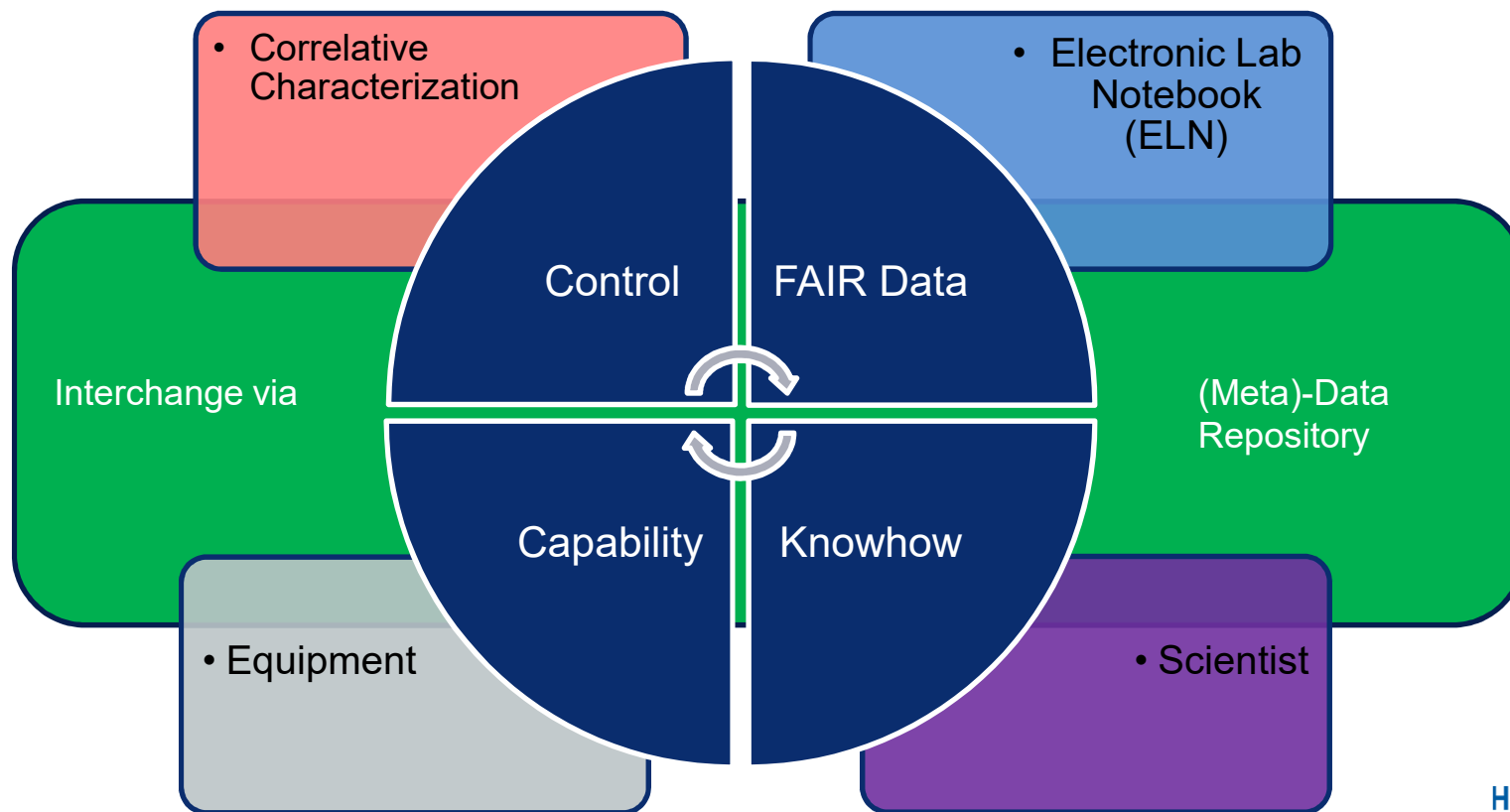Simplified Universal Metrology Process for Samples

Research Question ➜ Answer
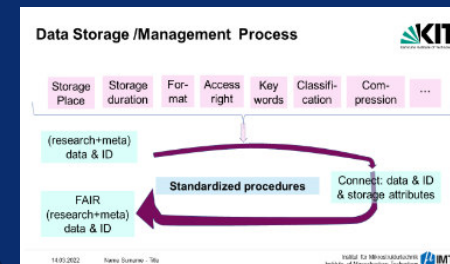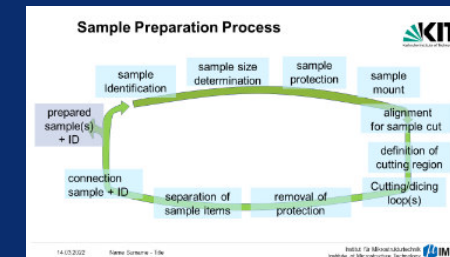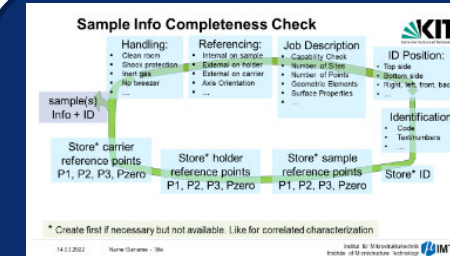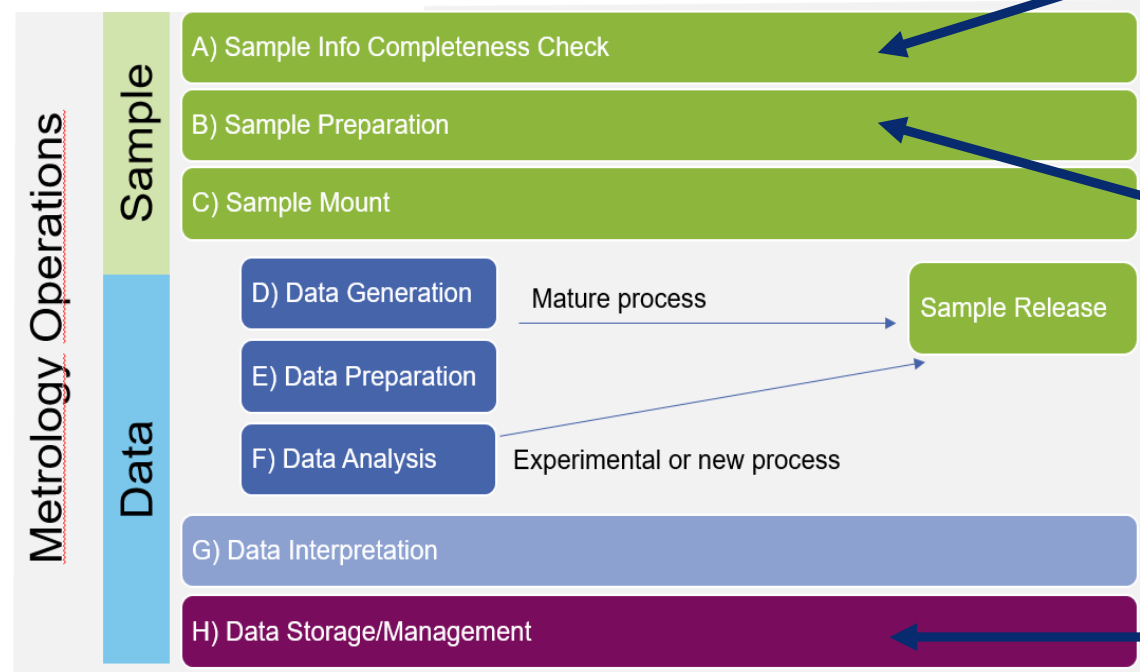
KIT Manufacturing Process

Simplified Universal Manufacturing Process for Samples

KIT Manufacturing Process

To get a General Idea

What an ELN should adress

Input from a Survey (a few future ELN Applicants, IMT only)

ELNs are compatible. Data exchange to other systems possible (common standard).
Map process sequence via "Process card" and display next steps
Different users must be able to add information about a sample/process/project or new process steps easily on site. How does version management work?
Quick and easy entry of process steps (e.g. using QR code)
Digital forms for process steps and samples. How to insert data from devices/systems?
Filtering by processes or parameters. Uniform tagging needed, link to ID number.
Link data sets (SEM, microscope, ...) automatically. As few clicks as possible for data backup. FAIR storage of secondary information
Browser-based (thus openly accessible on all OS)
Sign off process steps by authorized person (compare signature and date in processing card)
Project mapping (background info on sample, accompanying documents "goods in / goods out")
Automatic time-of-use recording
Automatic mails to next processor
Integration of FAQs, manual, possibly learning videos for basics, device-specific
Guest account with few queries/simple "manual" data entry at facility/device.
Bundling of user data and simplified user administration as additional task

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KIT Manufacturing Process

From Simple Process Flow to ELN

Lars Griem, IAM   Martin Starmann, IBCS

What else
- Specifications
- Standard Operating Procedures
- User Instructions
- Safety Data Sheets
- Manuals
- Training Docs
- Custom Tools
- Automation Programs
- Custom Carrier
- Device Maintenance Plan
- …

Total: >80 pages for a simple 3 step process

Issues addressed at KIT

Common Mechanical Interface
- Challenge: not available for many Devices
- Solution: 3D printed Interposers for quick Adaptation

Meta Data Collection
- Challenge: some Devices have no Meta Data available
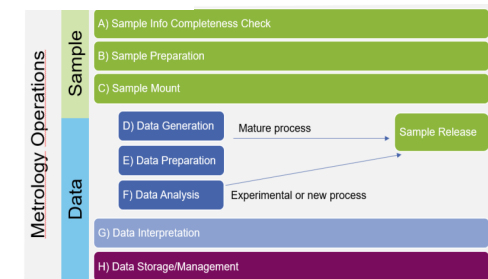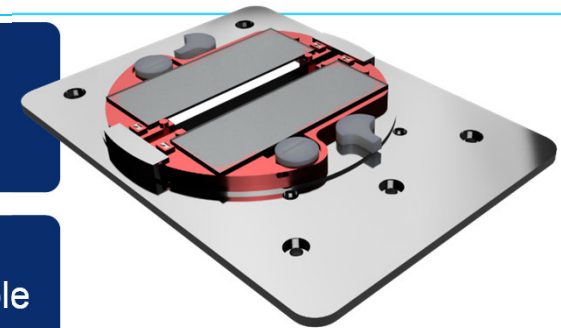- Solution: Custom SW to read Windows Handles

Network Connection
- Challenge: Standard is shifted from IPv4 to IPv6
- Solution: SCC Support to migrate Devices

Universal Metrology Process Description
- Challenge: versatile but detailed Description
- Solution: Process Flow developed within MDMC

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Issues to be addressed …

… by Helmholtz and beyond

Operating System Software Maintenance
- Challenge: Device SW Upgrade not synchronized
- Solution:

Transfer Process Knowledge from User to ELN
- Challenge: Hundreds of Steps, individual Knowhow, little Resources
- Solution:

Standardized PIN Generator
- Challenge: Diverse Requirements
- Solution:

Standardized Process Description
- Challenge: Who is defining the „Standard"
- Solution:

?

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Top Five Issues

1. Commitment that Infrastructure Development **is** Scientific Work. Even without any Publication.

2. Clever Strategy to separate Relevant Data from Total Data without Information Overflow

3. Protection of Knowledge/IP, secured Data Exchange

4. Local Resources for the Lab specific ELN Setup

5. Money to run Infrastructure beyond next POF Evaluation

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Resume´

Pros	Cons
■ Automation supports Reproducible Results	■ Forced to stay with SW (see Windows)
■ Documentation Standards to search for Experiments	■ High Level of Maintenance for HW/SW
■ More Time for Trials	■ Efficiency ≠ Scientific Quality
■ Knowledge Base for AI	■ Total Transparency: Dream … or Nightmare

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Outlook

- We are getting closer

- We will go on

- We might accelerate

- We should

Use coin to rub gently.
Avoid waste. Help to make the world a better place.

Scientists are liable for dreams that don't come true due to misuse, lack of productivity, delay
or any other shortcomings related to individual scientific work.

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The End

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