Sicherheit in Technik und Chemie

The intersection between Materials Science Engineering and Semantic Web

Andre Valdestilhas, Thomas Hanke, Thilo Muth, Bernd Bayerlein, Ghezal Ahmad Jan Zia, Benjamin Moreno Torres, Christoph Völker

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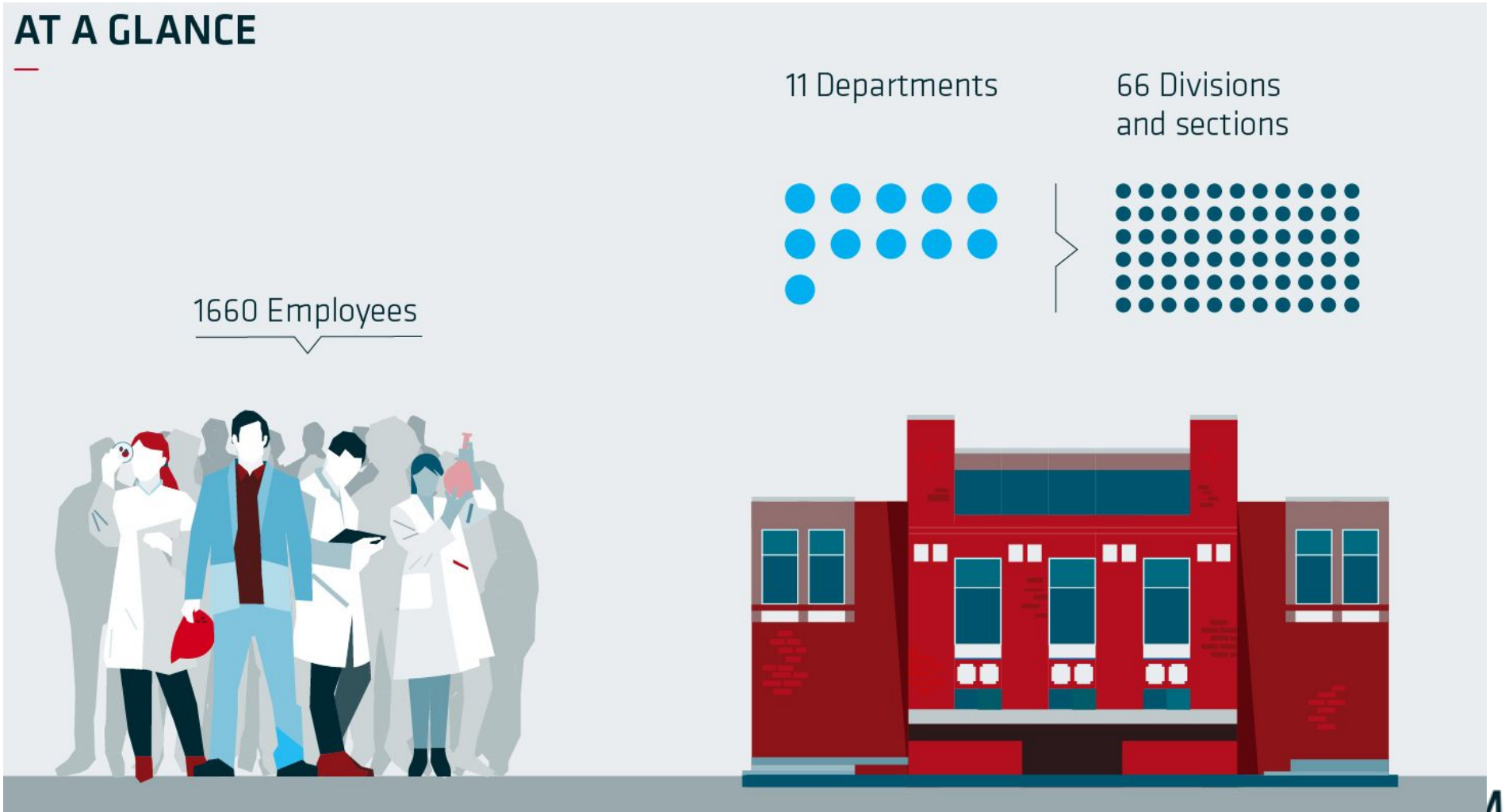
Outline

- BAM
- Motivation
- State of the art
- MSE ⋂ SW at BAM
- Conclusion

Federal Institute for Materials Research and Testing (BAM)



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Bundesanstalt für
Materialforschung
und -prüfung

- eScience group S.3
- Active since 2020
- > 20 employees
- National and International activities

Fraunhofer MATERIALS

MATERIALDIGITAL

Mat-O-Lab

- Research
- Coordination & Consultancy

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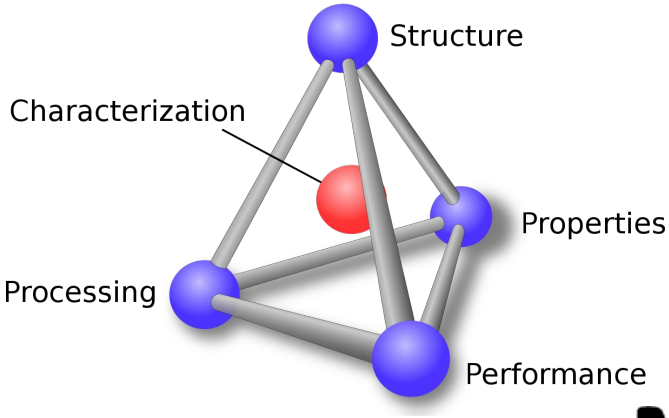
Materials Science Engineering and Semantic Web



Materials Science Engineering

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Mat-⏻-Lab

W3C Semantic Web

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Research Questions

RQ1. What are state-of-the-art approaches in MSE using SWT?

RQ2. Which SWT are applied in MSE?

RQ3. Does SWT influence the quality of an MSE experiment?

RQ.4 What are the open challenges on the intersection between MSE and SWT?

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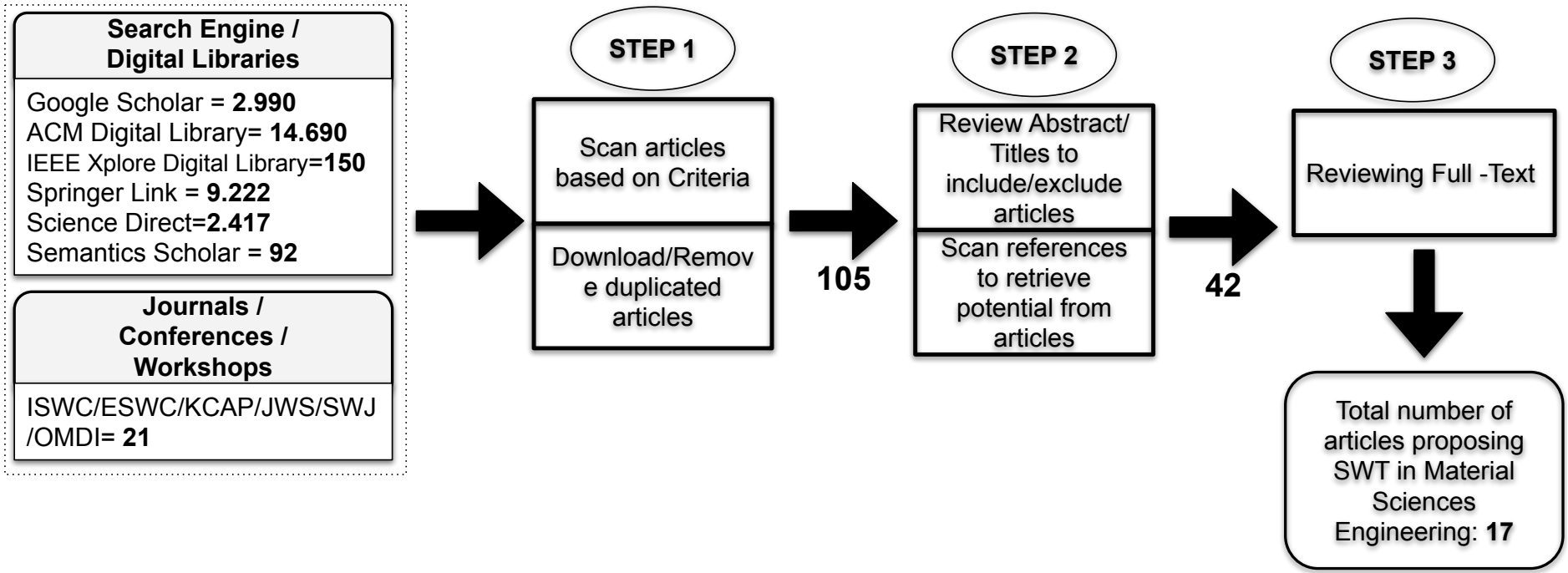
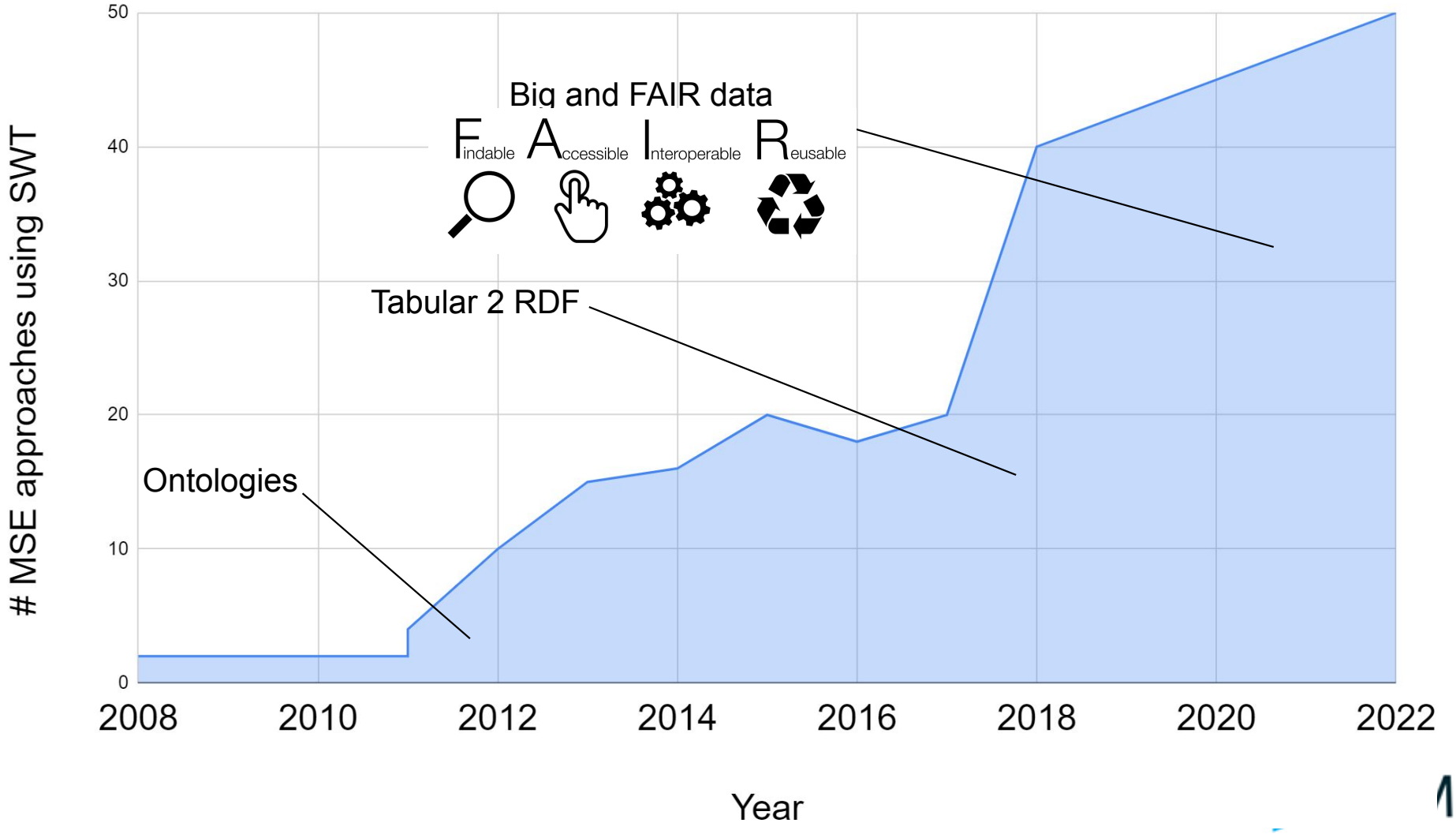
State of the art

RQ1. What are state-of-the-art approaches in MSE using SWT?

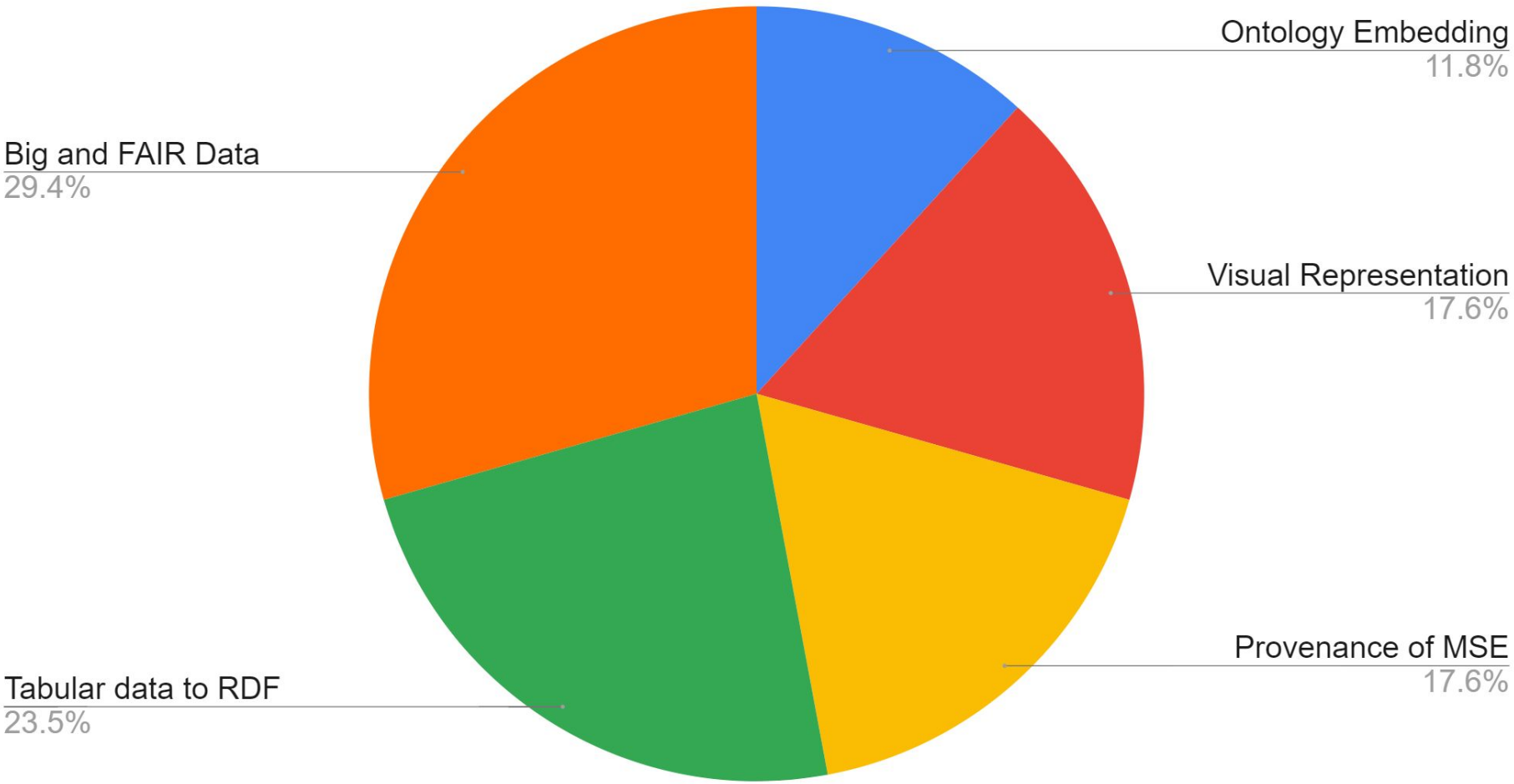


MSE ⋂ SWT x year



SWT in MSE in percentage

RQ2. Which SWT are applied in MSE?

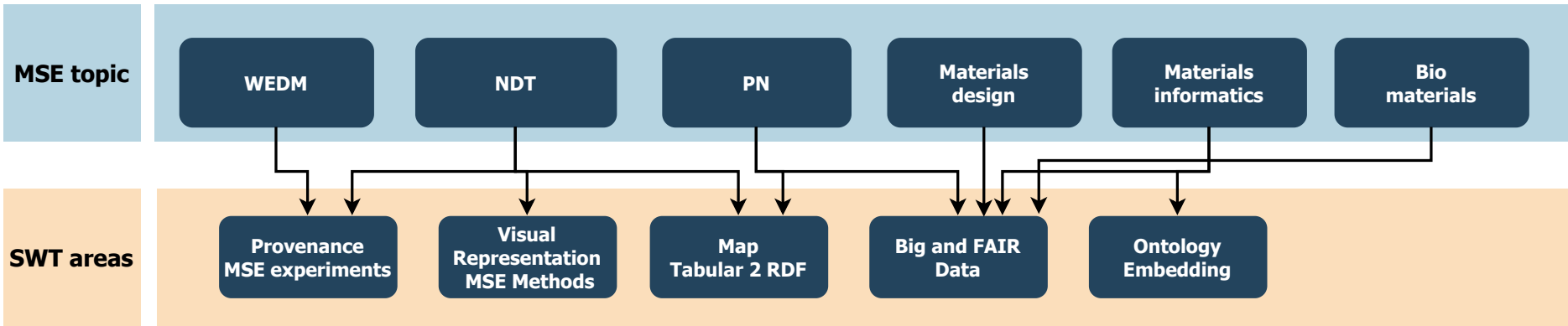


Classification

Open challenges in common

Example:

- Intersection of Big and FAIR Data with Materials design, Polymer Nanocomposites, Materials informatics, and Bio Materials
- On the other hand, there are MSE areas that need only provenance of MSE experiments (WEDM)



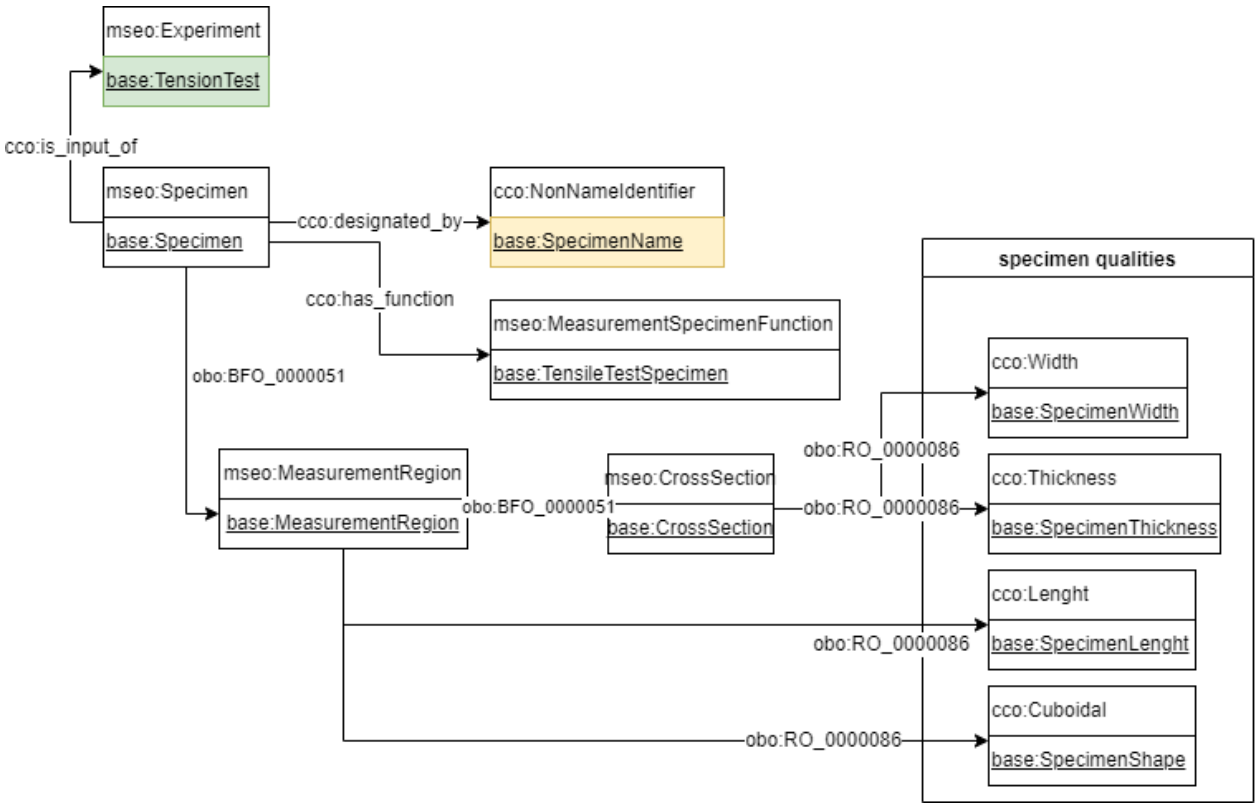
Polymer Nanocomposites (PN), Wire Eletrical Discharge Machining (WEDM),Non-Destructive Testing (NDT)

Challenges at BAM

MatVis (RQ3, RQ4)

Visual Representation of MSE Methods

- A Framework to Visually Represent MSE Methods and RDF Knowledge Graph Creation



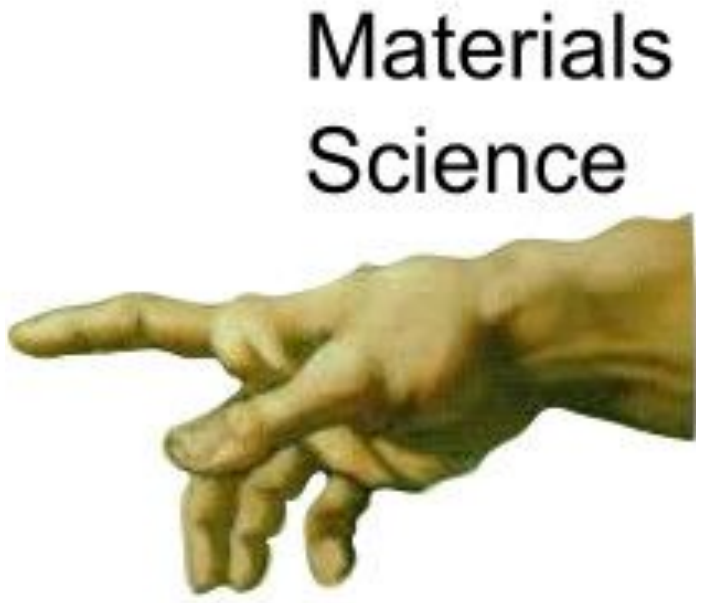
Challenges at BAM

NaturalMSEQueries (RQ3,RQ4)

- Natural Language Processing applied to query MSE data easier than SPARQL queries

NLP

NaturalMSE Queries



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Challenges at BAM

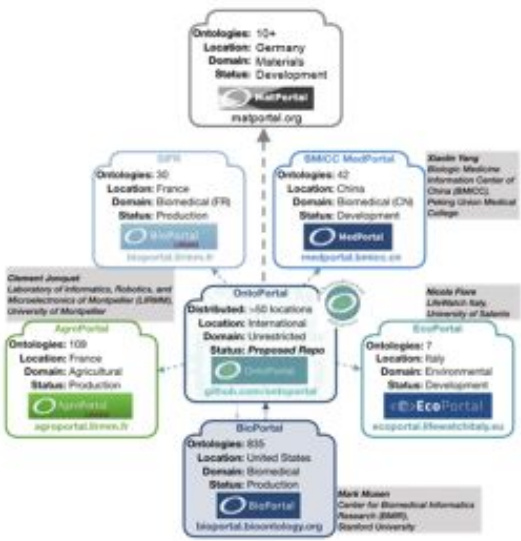
MatPortal[1] (RQ3, RQ4)

MatPortal: the first public ontology repository for the Material Sciences

Collaboration with OntoPortal Alliance / Stanford University

- Key component in the Mat-o-Lab ontology development workflow
- Shared repository for material science, avoiding duplication and loss of valuable work
- Providing a common collaboration and publishing system for ontologies

Fraunhofer MATERIALS



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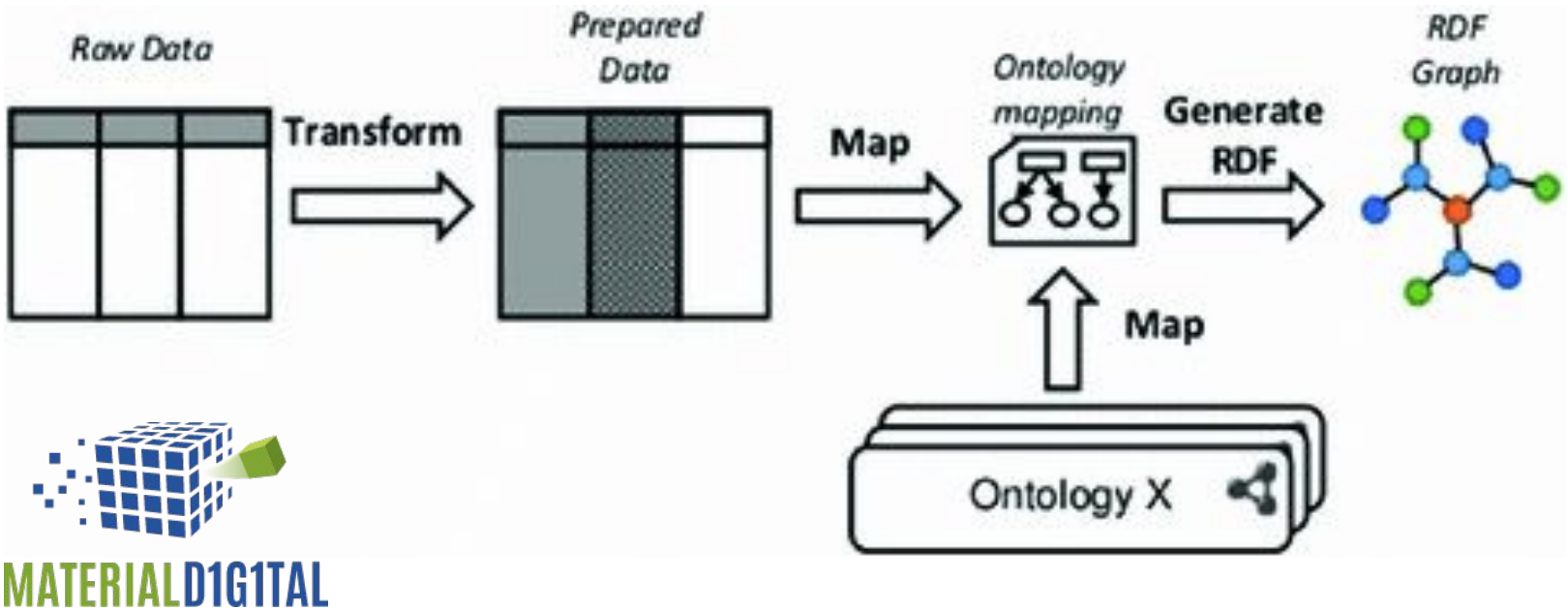
[1] https://matportal.org/

Challenges at BAM

LebeDigital[2]

- RDF Graph to store MSE data provenance from experimental data to model prediction



Sukhobok, Dina, et al. "Tabular data cleaning and linked data generation with Grafterizer." *European Semantic Web Conference*. Springer, Cham, 2016.

[2] BMBF-funded - https://material-digital.de/project/3

Challenges at BAM

Sequential Learning App for Materials Discovery - SLAMD [Völker et al. 2021][3] (RQ3, RQ4)

- **Ontology Embedding** helping to improve the the prediction of ideal material candidates
- Mapping Tabular data to RDF
- Machine Learning
- Acceleration:
  - **Before**: 82 … 480 Years
  - **After**: 45 … 630 Days

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[3] https://slamd-web.herokuapp.com/

Conclusion

- Detailed a systematic literature review of MSE using SW
- Illustrate the impact of applying SWT to MSE
- Present specific open challenges on the intersection between MSE and SWT
- Next steps (elaborate new approaches based the open challenges and the State of the art)

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Thanks!

Contact: Andre Valdestilhas
email: andre.valdestilhas@bam.de
web page: bam.de/e-science
twitter: @BamEscience
Link to the presentation: https://tinyurl.com/andrelswt2022

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