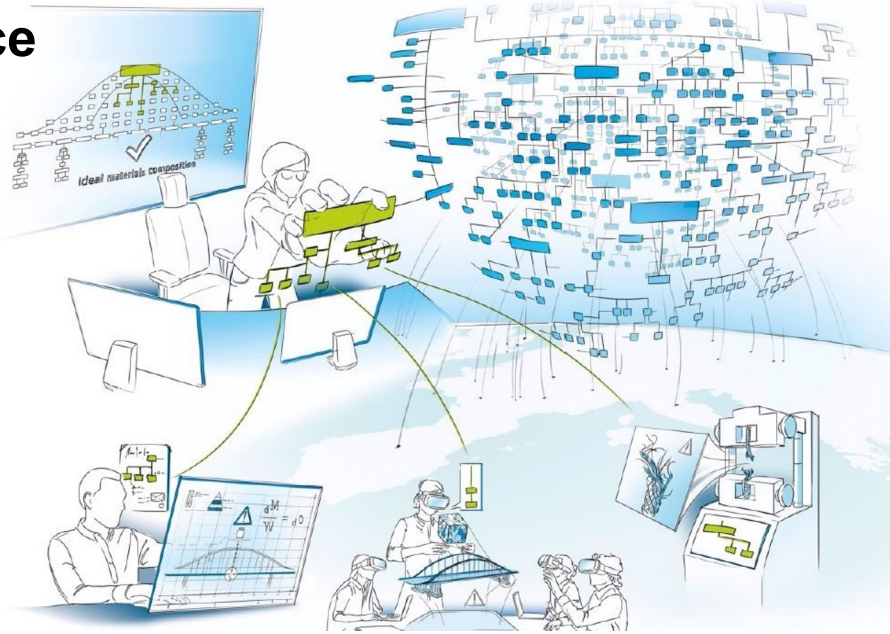
Applying Metadata Management

Extraction, Mapping & Visualisation

NFDI-MatWerk Conference

| Siegburg, 27.-29.06.23



Workshop Team:

Ajay Kirar
Benedikt Heinrichs
Elias Vitali
Gulzaure Abdildina
Reetu Joseph
Rossella Aversa

Agenda

- Introduction
- Demo: Semantic Metadata Extractor
    - Q/A session
- Introduction to FIB/SEM Tomography (PP13)
- Demo: Metadata Extraction & Mapping with the new interface
    - Q/A Session
- Demo: Metadata Visualisation
    - Q/A Session
- Wrap-up

Introduction

Aim of the workshop

To demonstrate how **Metadata Management** can be **applied** in practical scenarios by way of **extraction, mapping and visualisation**, which would ease the task for researchers by **decreasing time and the manual effort** needed.

Marktplatz

- Posters:
  - Metadata Extraction Tool and Schema Mapper for Scanning Electron Microscopy (SEM) images (Elias)
  - Semantic Metadata Extractor (Benedikt)
- Live demos
  - Demonstration of Automatic Metadata Extraction and Mapping for SEM Images (Elias & Ajay)

Demo: Semantic Metadata Extractor

Benedikt Heinrichs, Sirieam Hunke

Introduction

- There is an ongoing task to transform research data to FAIR Digital Objects (FDOs)
- These FAIR Digital Objects contain
  - The Digital Object (research data)
  - Metadata about the Digital Object
  - Some Service Interfaces
  - A Persistent Identifier
- The big point we focus on here today is metadata

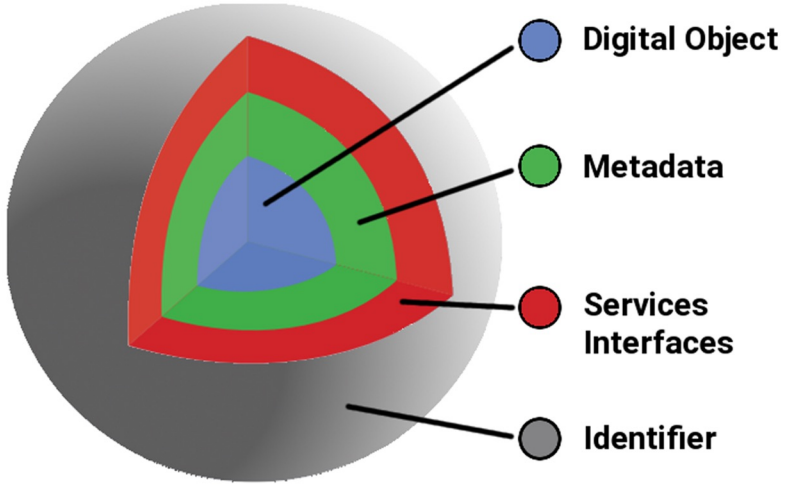
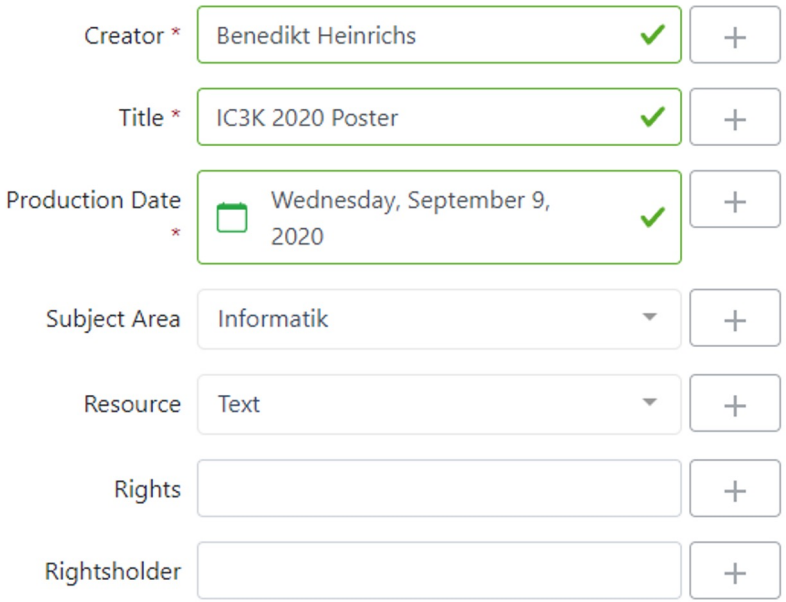


Image from "Digital Objects – FAIR Digital Objects: Which Services Are Required?", located at: https://datascience.codata.org/articles/10.5334/dsj-2020-015/

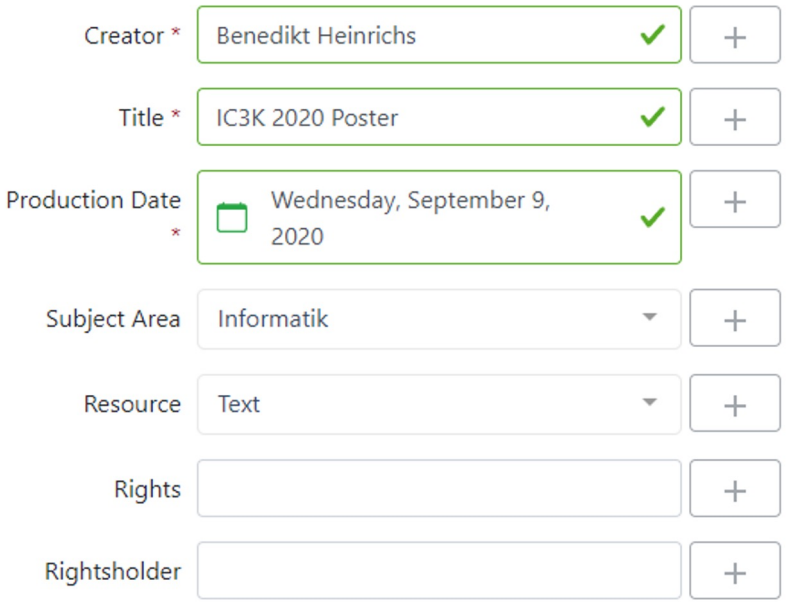
Metadata

- Why Metadata?
  - Describing the information surrounding the generation of a research item
  - Example: Describing a research experiment, the time it took place, etc.
- What Metadata?
  - Administrative: e.g. location or rights
  - Structural: provenance information
  - Descriptive: who, when or what
  - Semantic: Formulated in RDF using ontologies and validated by SHACL (W3C standard)
- How Metadata?
  - Manually input
  - Automatically generated during an experiment



Manual Metadata Input

- Administrative and Structural are usually fairly simple to automatically determine
  - e.g. a platform which manages metadata should be able to be aware of these types of metadata
- Descriptive metadata, however, currently mostly needs to be entered manually
  - This is usually a tedious and time-consuming task
  - A goal of RDM is to make the research process easier and not to create additional hurdles
    - Thankfully, the research data itself a lot of the time brings a subset of the necessary descriptive metadata with itself



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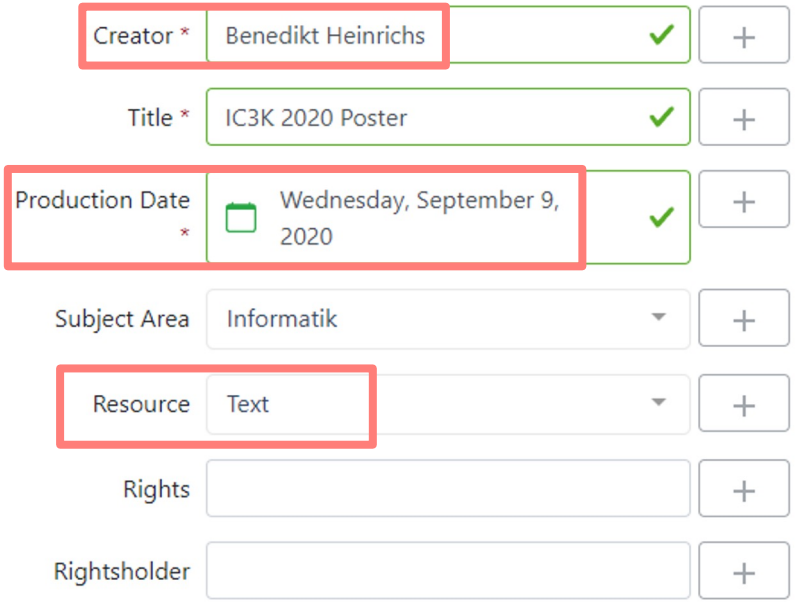
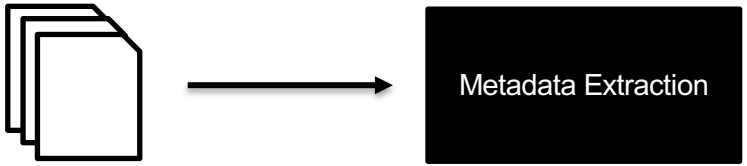
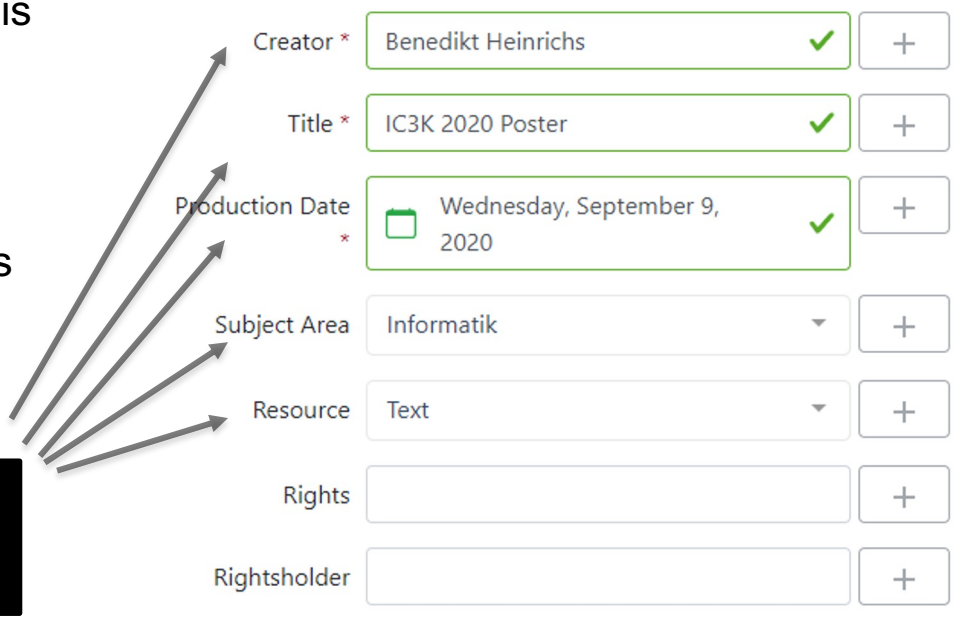


Motivation for Semantic Metadata Extraction

- We want to know what our research data is about
- We want to provide the most detailed information about the content of our research data
- We want to spend only as much time as is necessary to input values into forms
- Proposition:



Research Data



Filled out Metadata

Result Motivation for Semantic Metadata Extraction

```
47        image:mode "RGB" ;
48        ebucore:hasFormat "JPEG" ;
49        ebucore:height "425" ;
50        ebucore:width "640" .
51
52    imageobject:apple rdfs:label "apple" ;
53        imageobject:count "6" .
54
55    imageobject:orange rdfs:label "orange" ;
56        imageobject:count "7" .
```

TestText.txt - Editor

Datei Bearbeiten Ansicht

```
Benedikt and Amin work in the same office.
David is eavesdropping their conversation.
David can also speak chinese and knows the characters '性格'.
```

```
68  <http://pikes.fbk.eu/#Amin> a <http://www.newsreader-project.eu/ontologies/PERSON> .
69
70  <http://pikes.fbk.eu/#Benedikt> a <http://www.newsreader-project.eu/ontologies/PERSON> .
71
72  <http://pikes.fbk.eu/#eavesdropping> rdfs:seeAlso <http://dbpedia.org/resource/Eavesdropping> .
```

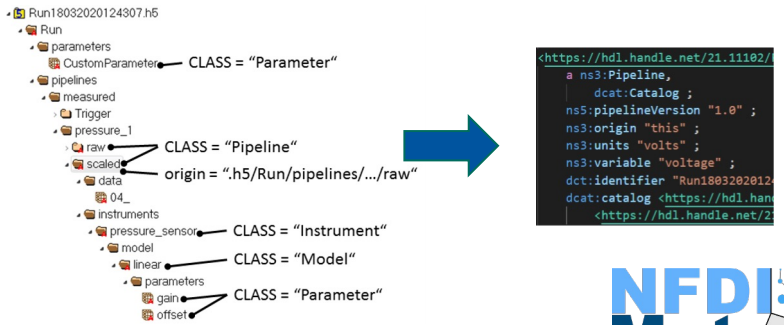
Prepare the deployment for production server

Refer to the product ticket for the description of the ticket.

- [ ] Update AutoSPInstaller.xml for installation
  - [ ] Check if there need to be seperate SP Installer xmls for the Farm join since there is only one farm.
  - [x] Check if we need a separate file. Set the secret keys and replace it with Consul values into the deployment script.
- [x] Detect why the error during installation "Previously installed Office 2019" (PreReqCheck) occurred
- [x] Parameter for the Installation => For Produktiv vs Dev
  - Create a parameter to filter (blacklist) steps
  - Add a json file with default values for config params, also secrets, check if this solves #322
- [ ] Make sure the production deployment is working
- [x] Put CoScInE DB creation into its own step and otherwise throw 3.02 out

Topic/600-productionDeployment

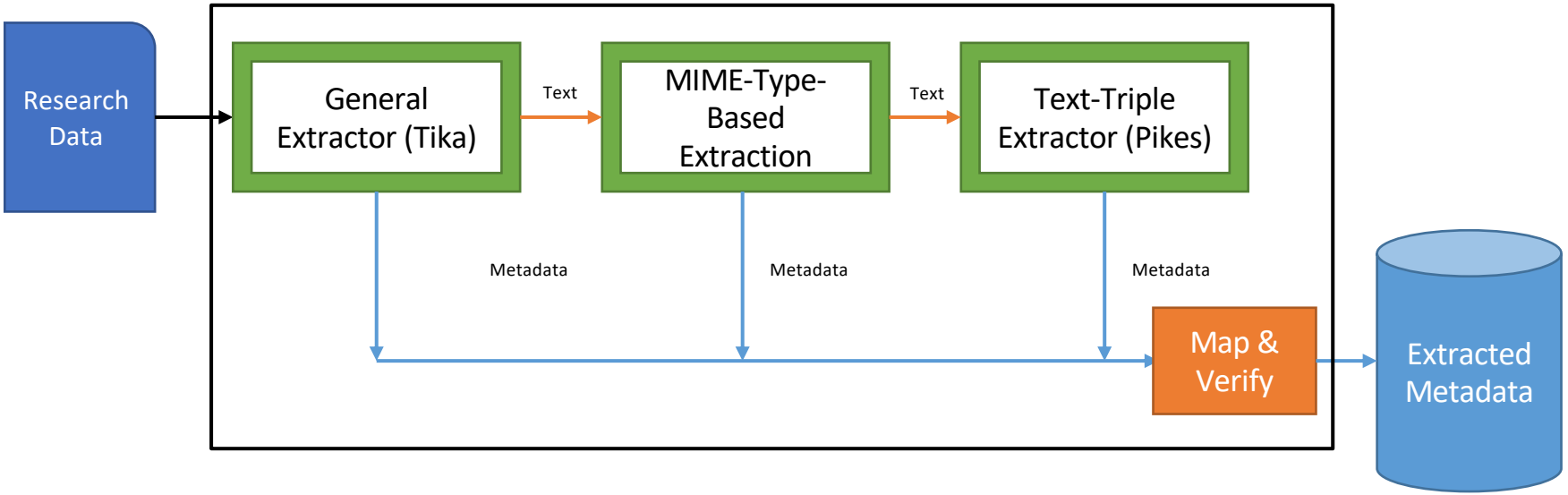
```
87
88    <http://pikes.fbk.eu/#installation> a <http://dbpedia.org/class/yago/Initiation107453195> ;
89        rdfs:seeAlso <http://dbpedia.org/resource/Installation_(computer_programs)> .
90
91    <http://pikes.fbk.eu/#json> rdfs:seeAlso <http://dbpedia.org/resource/JSON> .
92
```



HDF5 File Structure

Metadata Extraction Pipeline

Metadata Extraction



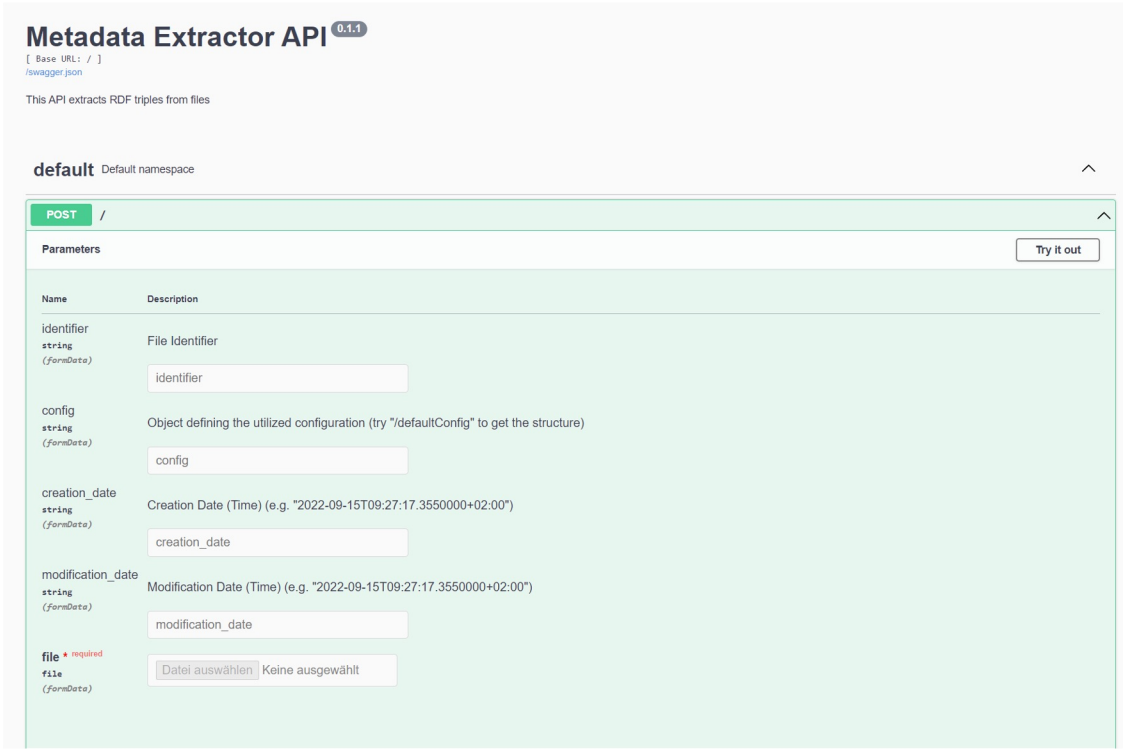
Heinrichs, B. ; Politze, M.
Moving Towards a General Metadata Extraction Solution for Research Data with State-of-the-Art Methods
12th International Conference on Knowledge Discovery and Information Retrieval, KDIR 2020, online, 2 Nov 2020 - 4 Nov 2020

Metadata Extraction Application – Features

- Dynamic Configuration
  - You can configure every extractor which shall be called and specify certain environment variables
- Registration of custom extractors
  - Once implemented, an extractor will listen to its registration method which can e.g. listen to certain MIME-Types like “image/png”
  - Custom extractors can be excluded from the default configuration, so that specific use cases can be proposed without impacting everything else
- Highly extendable
  - By being open source, this application is easily extendable to different areas
    - https://git.rwth-aachen.de/coscine/research/metadataextractor

Metadata Extraction Service

https://metadataextractor.otc.coscine.dev/



Example Results – Object Detection

```
47          image:mode "RGB" ;
48          ebucore:hasFormat "JPEG" ;
49          ebucore:height "425" ;
50          ebucore:width "640" .
51
52      imageobject:apple rdfs:label "apple" ;
53          imageobject:count "6" .
54
55      imageobject:orange rdfs:label "orange" ;
56          imageobject:count "7" .
```

Example Results – Text

TestText.txt - Editor

Datei Bearbeiten Ansicht

```
Benedikt and Amin work in the same office.
David is eavesdropping their conversation.
David can also speak chinese and knows the characters '性格'.
```

```
68    <http://pikes.fbk.eu/#Amin> a <http://www.newsreader-project.eu/ontologies/PERSON> .
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71
72    <http://pikes.fbk.eu/#eavesdropping> rdfs:seeAlso <http://dbpedia.org/resource/Eavesdropping> .
```

Example Results – Image to Text

Prepare the deployment for production server

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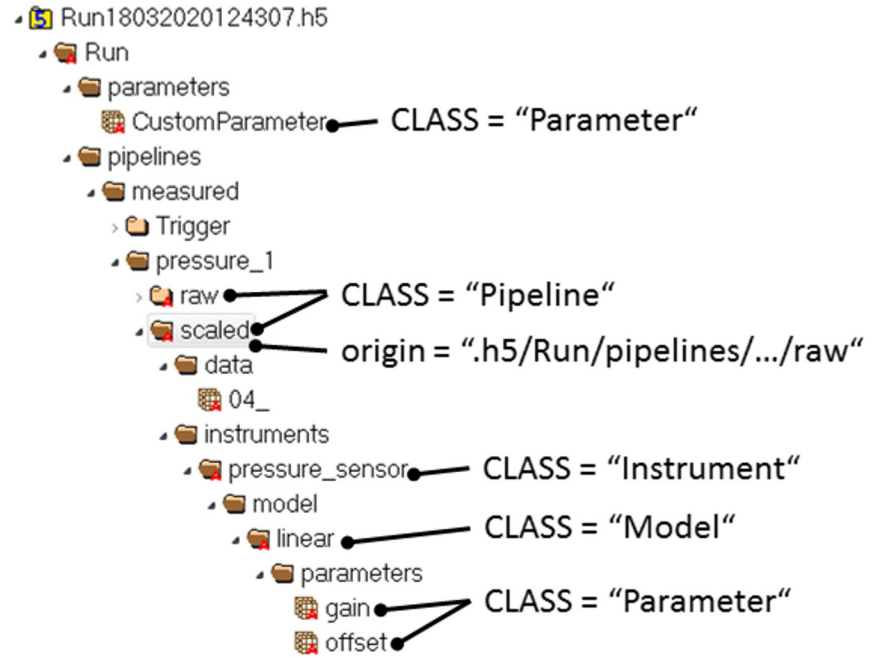
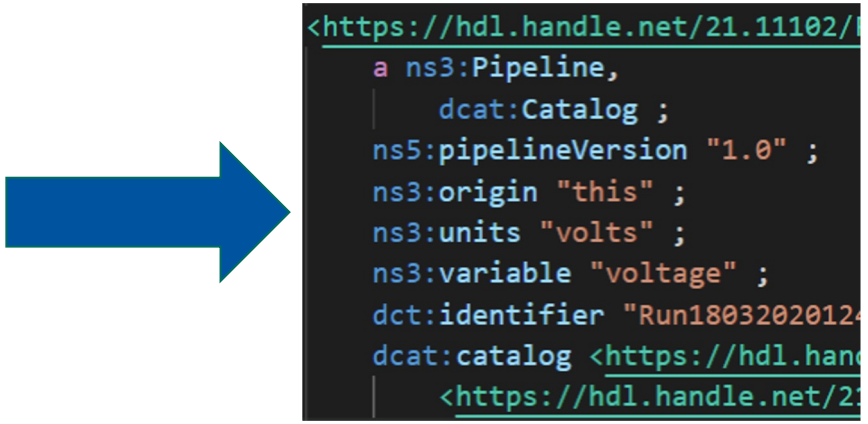
Topic/600-productionDeployment

```
87
88    <http://pikes.fbk.eu/#installation> a <http://dbpedia.org/class/yago/Initiation107453195> ;
89        rdfs:seeAlso <http://dbpedia.org/resource/Installation_(computer_programs)> .
90
91    <http://pikes.fbk.eu/#json> rdfs:seeAlso <http://dbpedia.org/resource/JSON> .
92
```

Example Results – Real Example with HDF5





HDF5 File Structure

Heinrichs, B. P. A. ; Preuß, N. ; Politze, M. ; Müller, M. S. ; *et al*
Automatic General Metadata Extraction and Mapping in an HDF5 Use-case
Proceedings of the 13th International Joint Conference on Knowledge Discovery, Knowledge Engineering and Knowledge Management

Metadata Extraction Service – Usage

Open Source

- Git Repo (Python Code): https://git.rwth-aachen.de/coscine/research/metadataextractor
- Docker Image: registry.git.rwth-aachen.de/coscine/research/metadataextractor:latest
- Demo: https://metadataextractor.otc.coscine.dev/
- Start adding your own extractor now by using Gitpod: https://gitpod.io/#https://git.rwth-aachen.de/coscine/research/metadataextractor

Metadata Extraction Service – Future Work

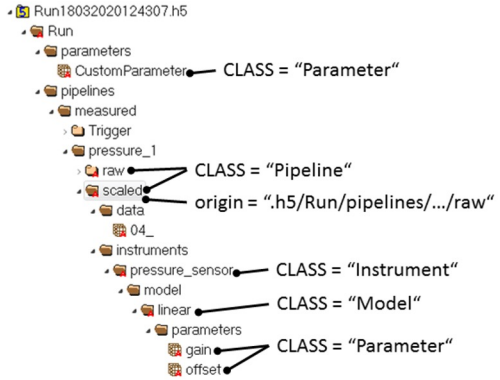
- Inclusion in research data management systems like Coscine
  - Automatically extract the metadata for research data based on a given configuration
  - Fill the metadata form automatically based on a templating engine
  - Make use of the extracted metadata in applications like “search”

- Utilize the extracted metadata to determine the similarity between research data when the MIME-Type is different (e.g. image with text vs. text file)
  - Making use of https://git.rwth-aachen.de/coscine/research/semanticsimilarity

- Improve the performance and make it better scale against big research data

Conclusion

- Today, I showed a look into our proposed solution of semantic metadata extraction
- It is a pipeline which takes research data and tries to describe the content as semantic metadata
- The usage has been demonstrated on different examples with a real-life use case as well



HDF5 File Structure

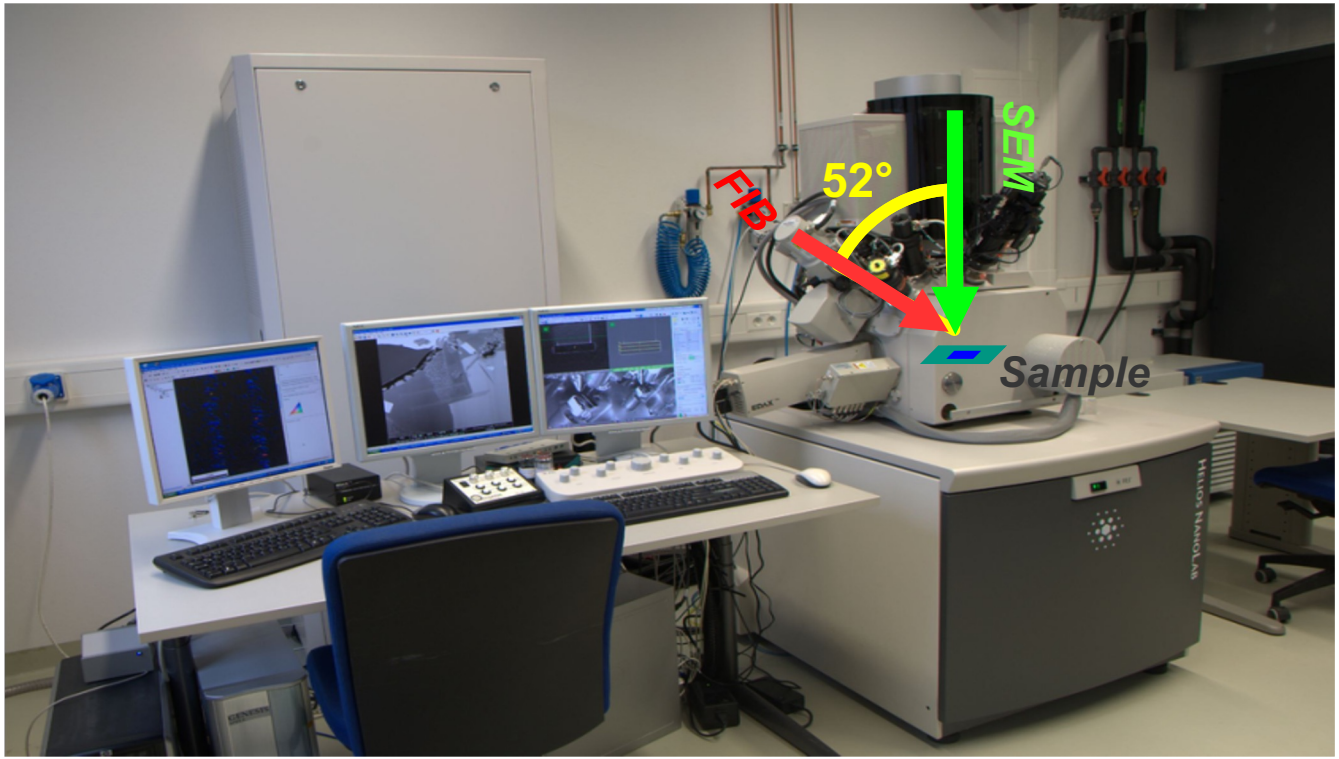
- Future work is being done to utilize this in real life applications

Q & A

Introduction to FIB/SEM Serial Sectioning Tomography (PP13)

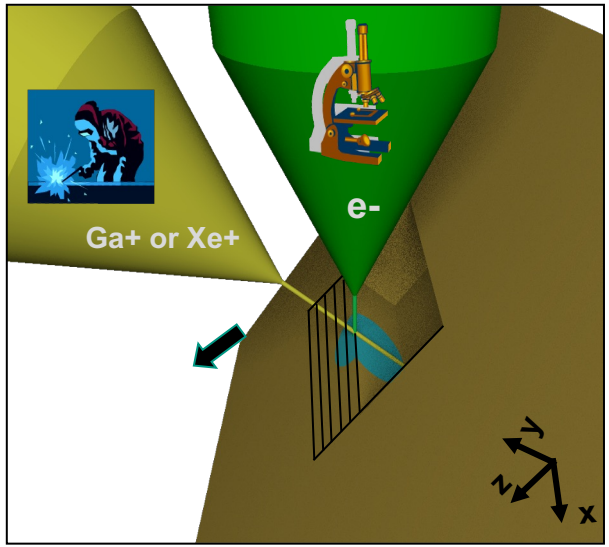
Reetu Joseph, Rossella Aversa, Christoph Pauly

FIB/SEM Serial Sectioning Tomography Apparatus

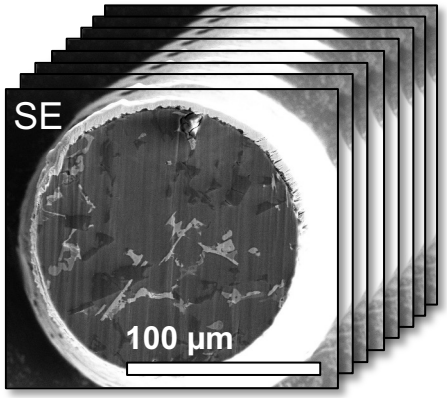


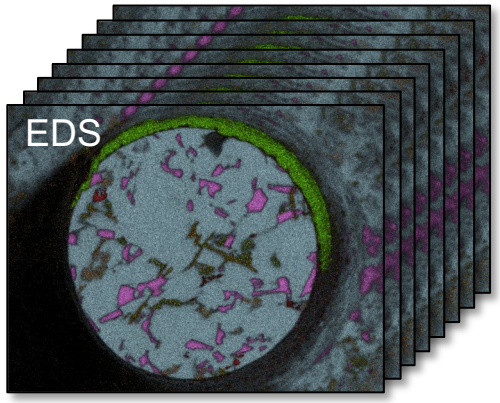
Courtesy: Christoph Pauly & Michael Engstler, Saarland University

I. Serial sectioning and multimodal imaging

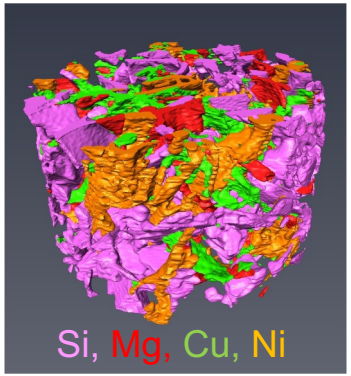


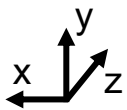
II. Image Processing and 3D reconstruction





2D image stack
(x-y-plane)

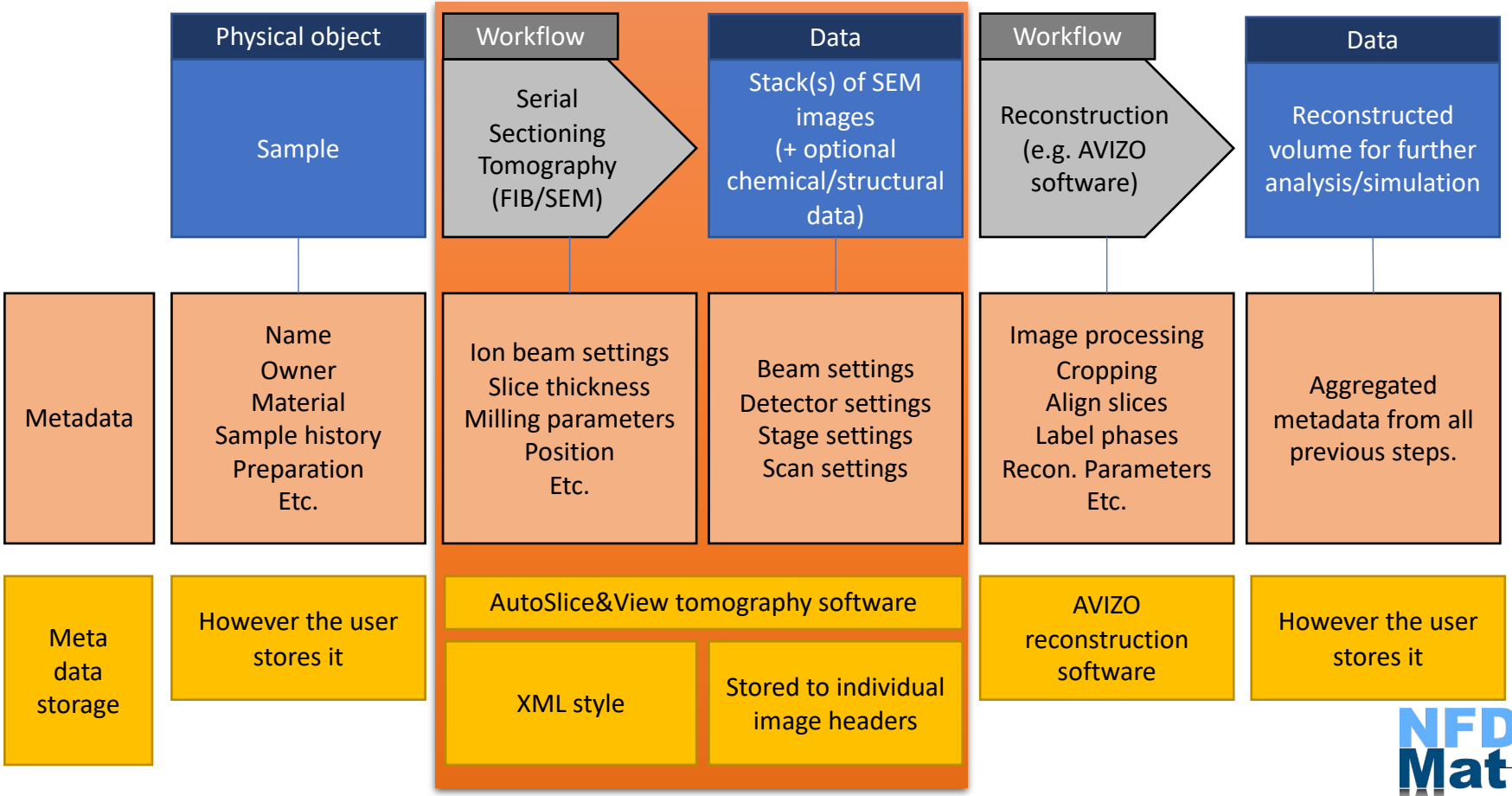




3D volume based
on EDS data (x-y-z)

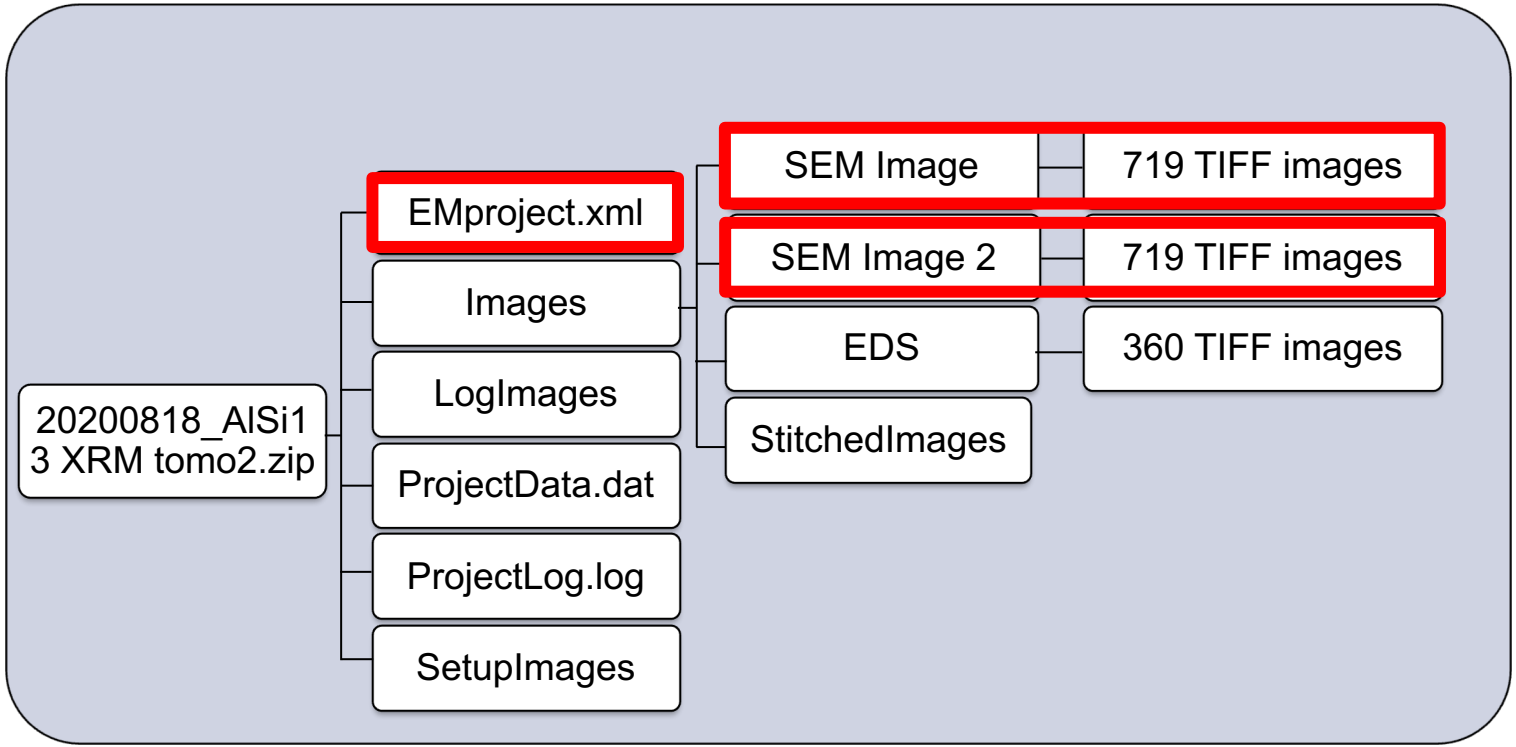
NFDI MatWerk

Courtesy: Christoph Pauly & Michael Engstler, Saarland University



Metadata Handling

Acquistion Data



Demo + Presentation: Metadata Extraction & Mapping – SEM/FIB Serial Sectioning Tomography

Elias Vitali, Ajay Kirar, Reetu Joseph, Rossella Aversa

Acquistion Data

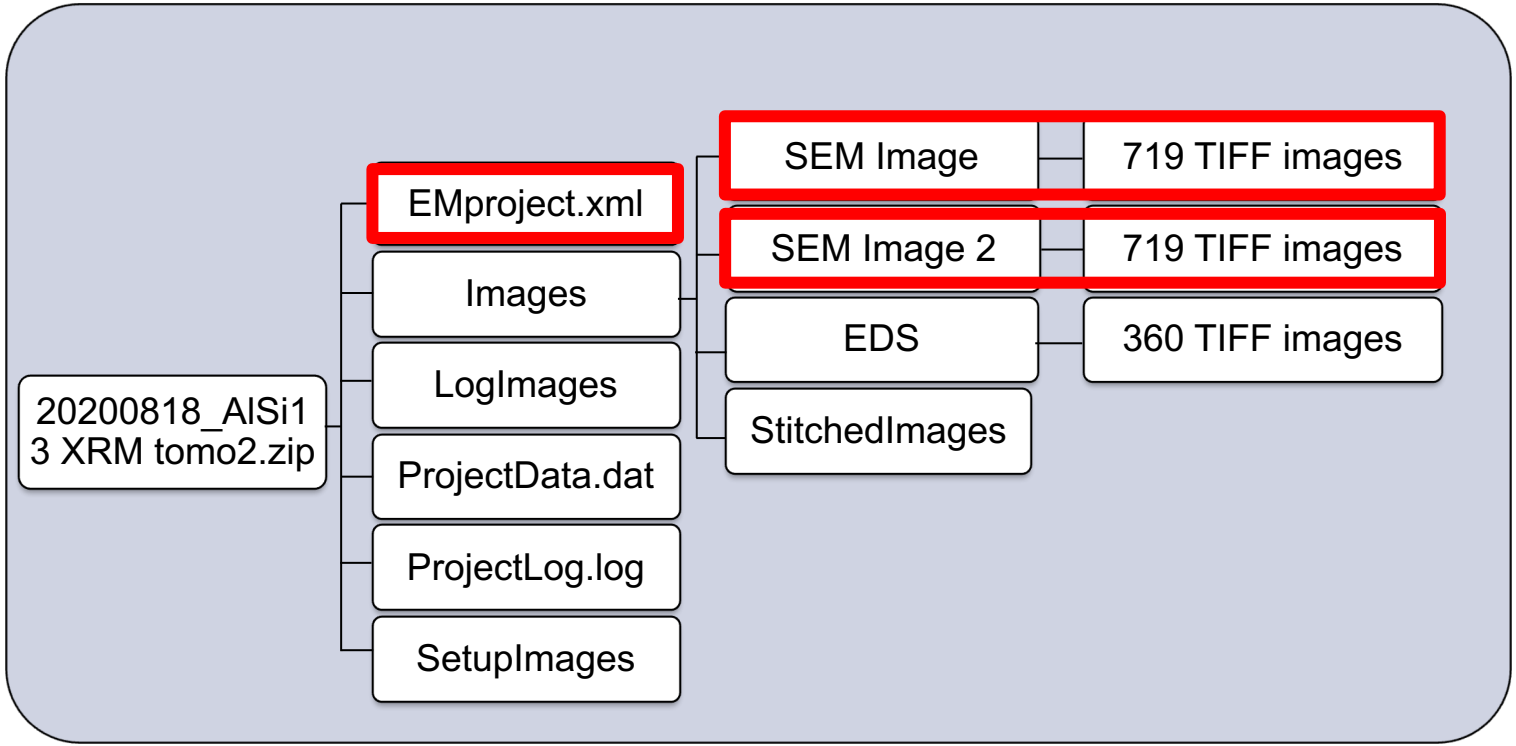
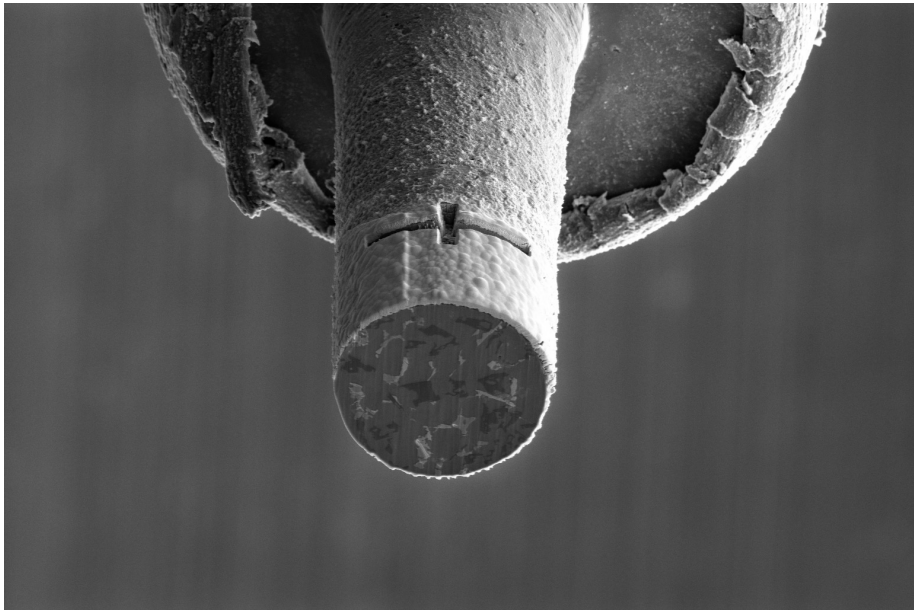


Image Metadata



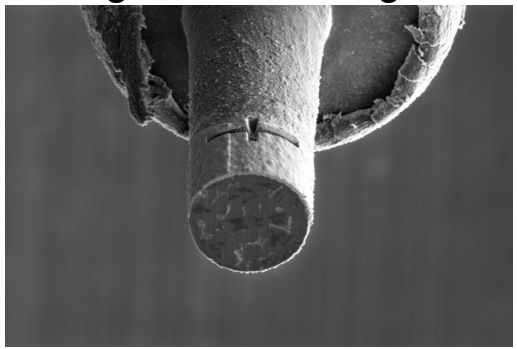
- Hidden in this image is a ton of metadata
- Need an efficient method to extract this metadata

Desired Result

- We want a metadata document that describes:
  - the acquisition;
    - each dataset;
      - each image.
- A schema dictates the format which this metadata document should take
  - This lets us ”map” the metadata

Process at a glance

1. Original TIFF image with all metadata



```
HV=15000
HFW=0.000592
VFW=0.000394667
WD=0.00402349
BeamCurrent=1.6e-009
```

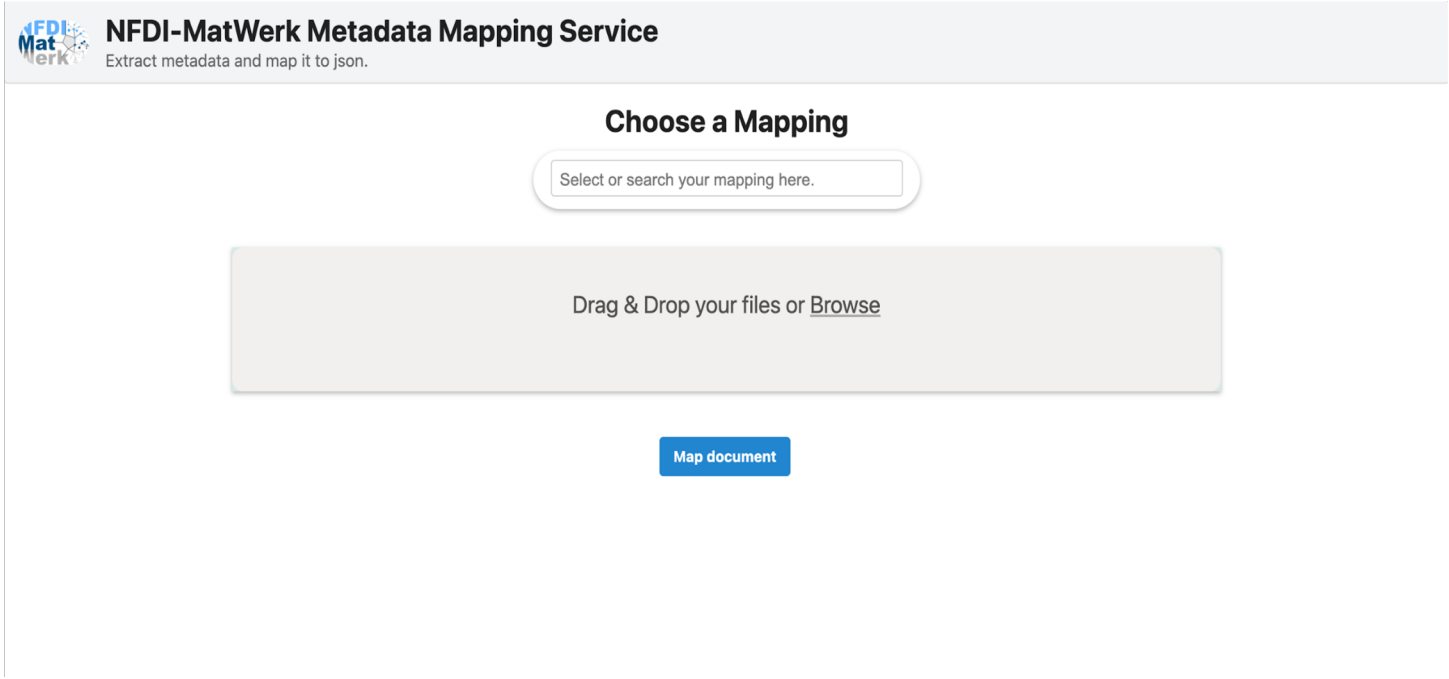
```
"acquisition.dataset.instrument.eBeam.accelerationVoltage.value":"Images.SEM Image.SliceImage.EBeam.hv",
"acquisition.dataset.instrument.eBeam.beamCurrent.value":"Images.SEM Image.SliceImage.EBeam.beamcurrent",
"acquisition.dataset.instrument.eBeam.scanRotation.value":"Images.SEM Image.SliceImage.EBeam.scanrotation",
```

2. Map file which translates original keys to schema keys

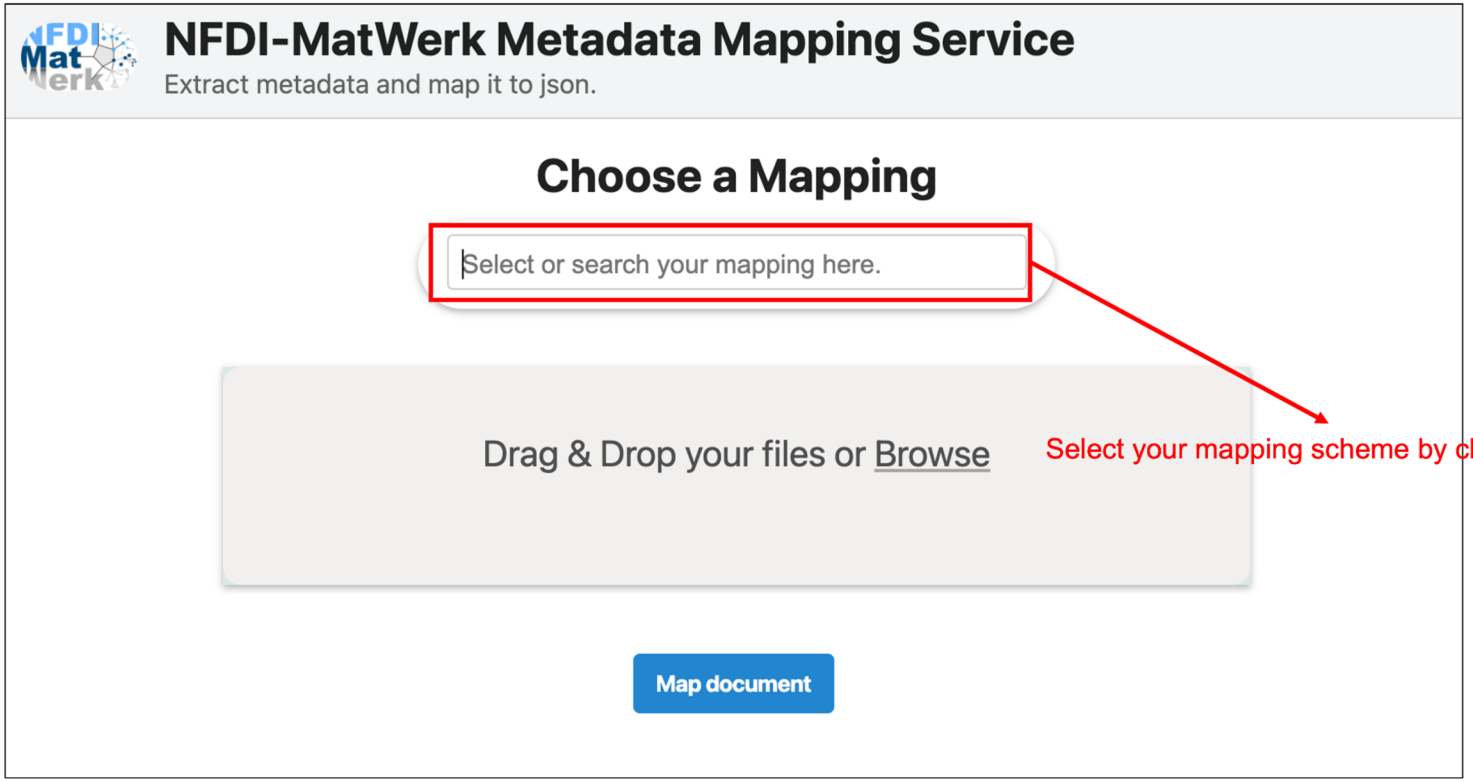
3. Formatted metadata document

```
{
    "acquisition": {
        "genericMetadata": {…
        },
        "dataset": [
            {
                "rows": "1",
                "columns": "1",
                "tileColumn": "0",
                "user": {…
                },
                "program": {…
                },
                "instrument": {
                    "beamType": "EBeam",
                    "spot": "1",
                    "eBeam": {
                        "accelerationVoltage": {
                            "value": "15000"
                        },
                        "beamCurrent": {
                            "value": "1.6e-009"
                        },
```

The Mapping Service



1. Choose the mapping scheme



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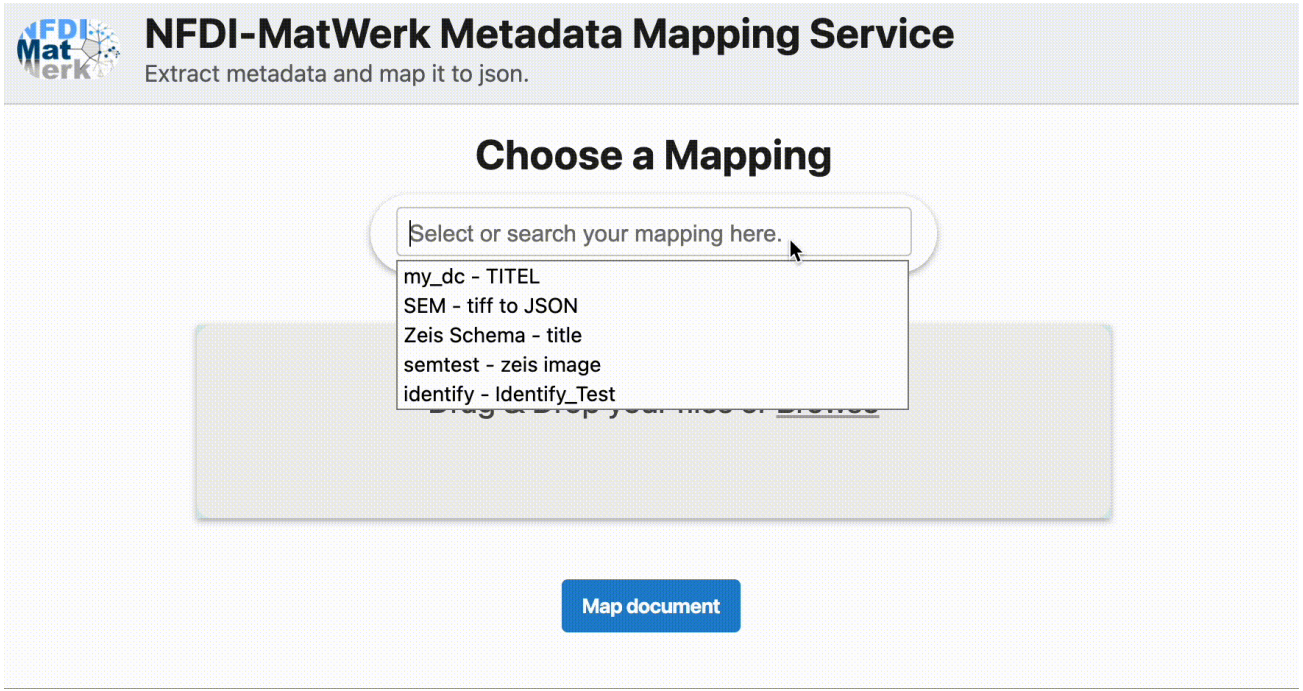
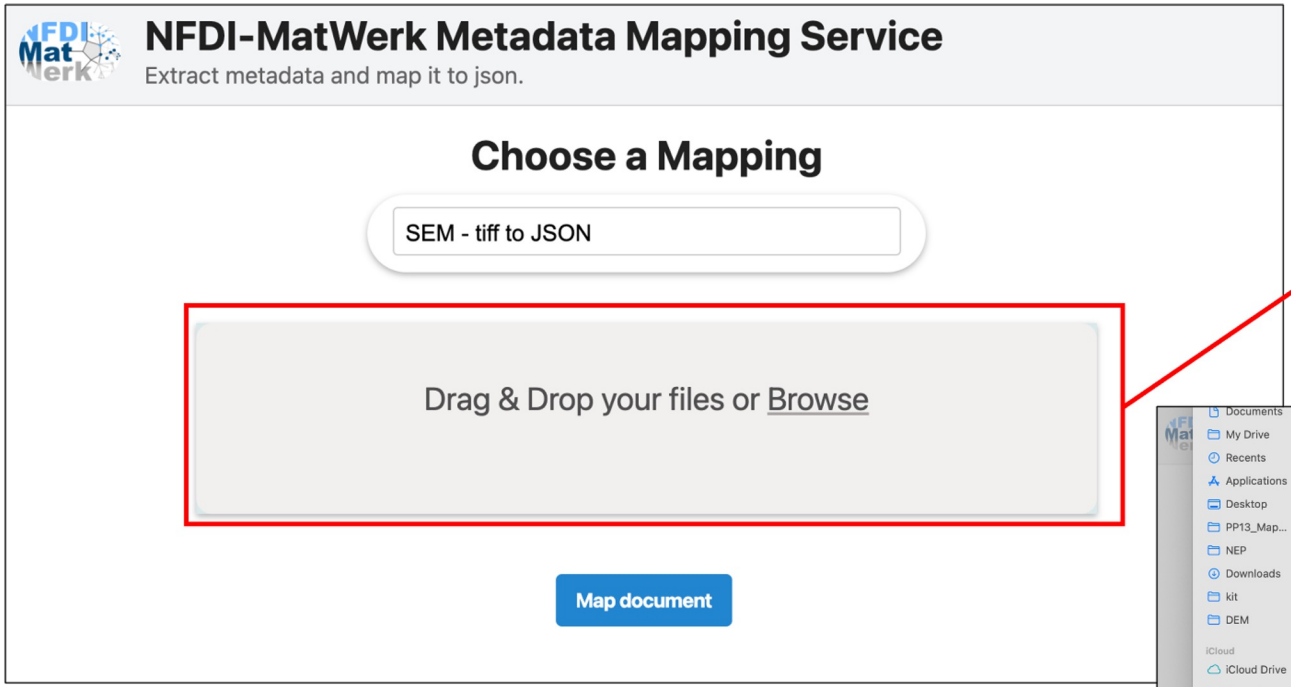
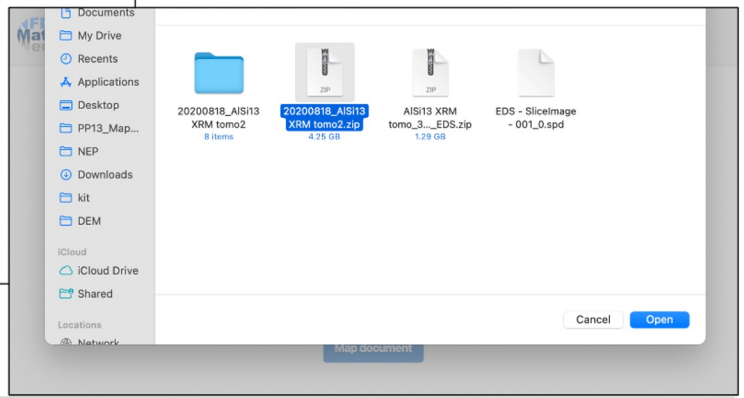


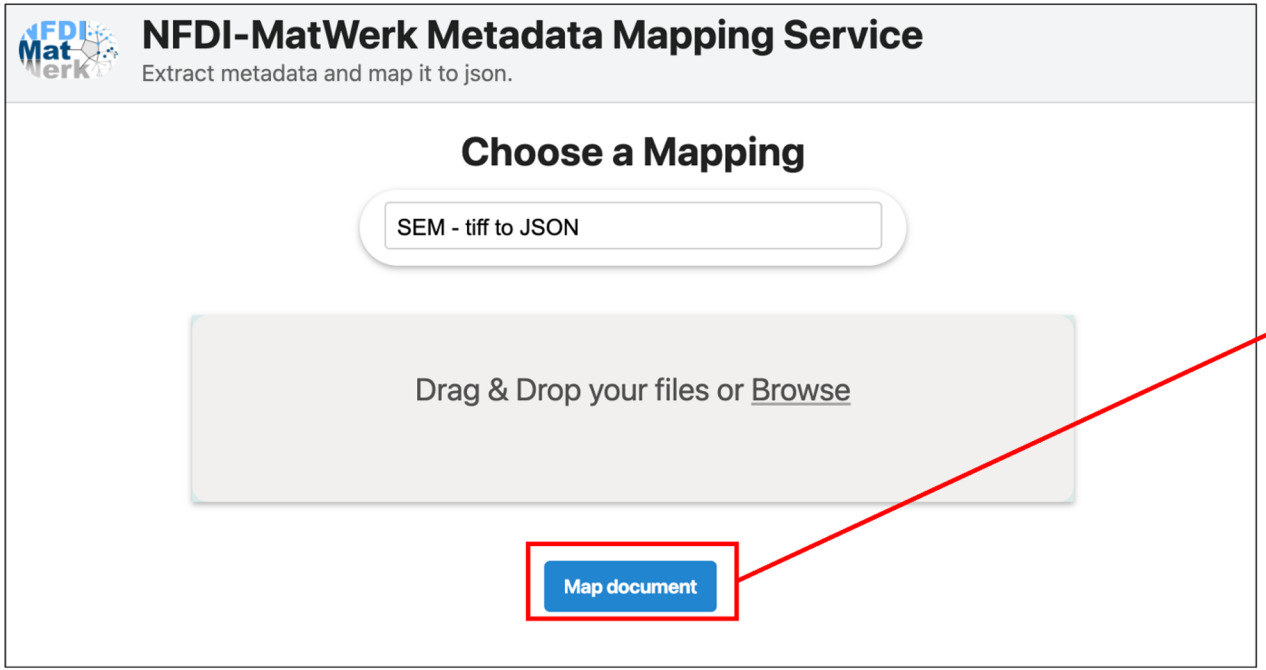
2. Uploading the dataset



Click on “Choose File” and upload the desired dataset



3. Map and download



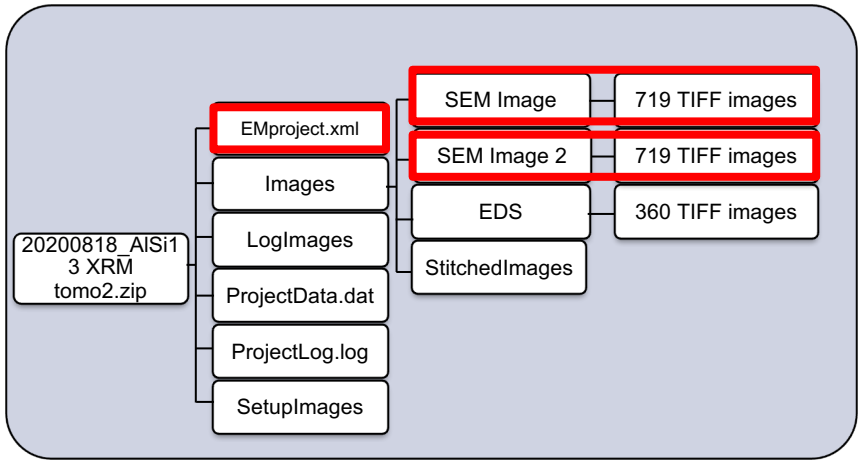
Click “Map document”. A download of the results file should automatically start, if it doesn’t, you can also click on the ”Download result” button which will appear after mapping.

4. Examine the results


```
{
    "acquisition": {
        "genericMetadata": {
            "program": {
                "programName": "Auto Slice & View 4",
                "programVersion": "4.2.1.1982"
            },
            "applicationId": {
                "identifierValue": "ASV"
            },
            "fileVersion": "1.2",
            "projectName": "20200818_AlSi13 XRM tomo2",
            "zCutSpacing": {
                "value": "2.0000000000000002E-07"
            },
            "numberOfCuts": "719",
            "pump": "TMP",
            "column": "Elstar",
            "source": "FEG",
            "eucentricWorkingDistance": {
                "value": "0.004"
            },
```

Summary

- Automatically extract data from hundreds of images in one swift process
- Reorganized metadata in a structured format according to a published schema




```
{
    "acquisition": {
        "genericMetadata": {
            "program": {
                "programName": "Auto Slice & View 4",
                "programVersion": "4.2.1.1982"
            },
            "applicationId": {
                "identifierValue": "ASV"
            },
            "fileVersion": "1.2",
            "projectName": "20200818_AlSi13 XRM tomo2",
            "zCutSpacing": {
                "value": "2.0000000000000002E-07"
            },
            "numberOfCuts": "719",
            "pump": "TMP",
            "column": "Elstar",
```

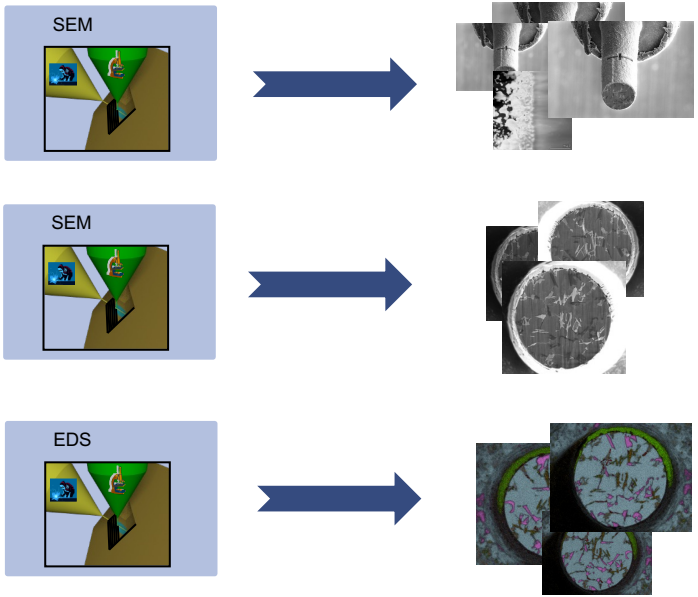
Q & A

Visual Analysis of complex metadata of SEM/FIB Tomography TIFF images

Gulzaure Abdildina, Rossella Aversa

Problem

Each experiment produces a large amout of data



Scientists need to:

- Analyze a large amount of experimental results.
- Monitor the experiment's progress for expected outcomes.
- Compare results from multiple experiments.

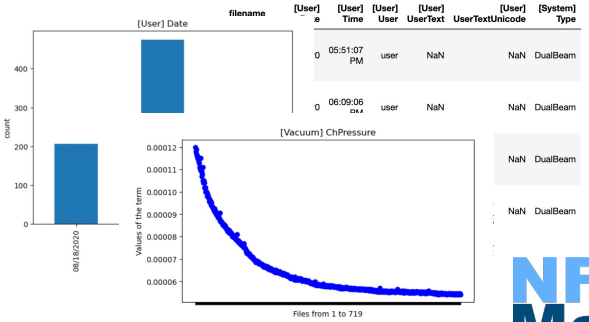
How can these processes be automated to facilitate the decision-making process?

Visual Analyzer

Python-based Jupyter Notebook which allows to:

- quickly overview metadata of SEM/FIB Tomography TIFF images
- visualize metadata for the analysis of experiment results -> makes complex data more accessible and understandable
- support scientists in accelerating decision-making processes

applying Visual Analyzer



Quick overview of the metadata

- Overall view of the metadata: statistics and common trends

	filename	user Date	user userName	program programName	spot	beamType	scan scanType	eBeam apertureSetting Size	accelerati
count	719	719	719	719	719	719	719	719	
unique	719	3	1	1	1	1	1	1	
top	SEM Image - SliceImage - 085.tif	08/19/2020	user	14.5.1.432	1	EBeam	EScan	4.53e-005	
freq	1	474	719	719	719	719	719	719	

4 rows × 75 columns

Quick overview of the metadata

Analysis of the metadata:

- Total number of metadata terms - 73
- Terms with constant values - 65
- Terms with changing values - 8 :
  - according to schema changing values can be 16

Quick overview of the metadata with changing values

Metadata with changing values

```
Data columns (total 9 columns):
 #   Column                  Non-Null Count  Dtype
---  ------                  --------------  -----
 0   filename                719 non-null    object
 1   stage StageX            719 non-null    float64
 2   stage StageY            719 non-null    float64
 3   stage StageTa           719 non-null    float64
 4   stage workingDistance   719 non-null    float64
 5   imaging driftcorrected  719 non-null    object
 6   vacuum chamberPressure  719 non-null    float64
 7   image specimenCurrent   719 non-null    float64
 8   images creationTime     719 non-null    object
```

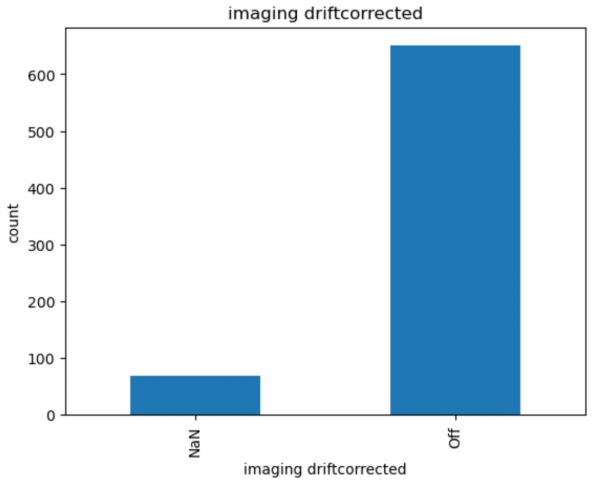
Overview of the values

filename	user Date	stage StageX	stage StageY	stage StageTa	stage workingDistance	driftc
SEM Image - SliceImage - 001.tif	08/18/2020	0.000225271	-0.00467317	0.336851	0.00402349	
SEM Image - SliceImage - 002.tif	08/18/2020	0.000225271	-0.00467317	0.336851	0.00402365	
SEM Image - SliceImage - 003.tif	08/18/2020	0.000225271	-0.00467317	0.33685	0.00402381	
SEM Image - SliceImage - 004.tif	08/18/2020	0.000225271	-0.00467317	0.336851	0.00402396	

Visualizing Metadata

Grouping images by *driftcorrected*:

- Metadata *driftcorrected* has two values
- We can also investigate how many and which images has missing values

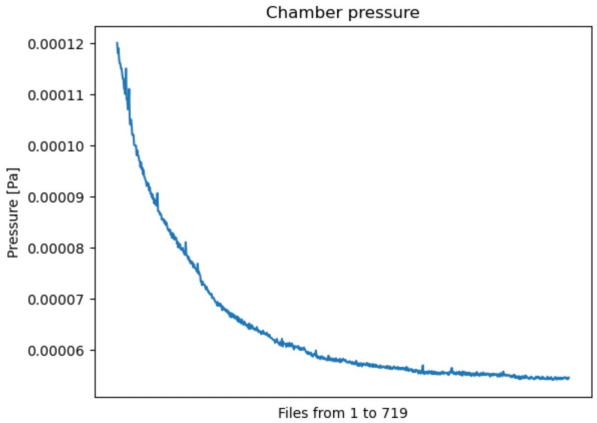


Images with missing *driftcorrected* values

	filename	imaging driftcorrected
673	SEM Image - SliceImage - 048.tif	NaN
101	SEM Image - SliceImage - 050.tif	NaN
5	SEM Image - SliceImage - 052.tif	NaN
107	SEM Image - SliceImage - 054.tif	NaN
205	SEM Image - SliceImage - 056.tif	NaN
717	SEM Image - SliceImage - 063.tif	NaN
629	SEM Image - SliceImage - 065.tif	NaN
551	SEM Image - SliceImage - 073.tif	NaN
701	SEM Image - SliceImage - 103.tif	NaN

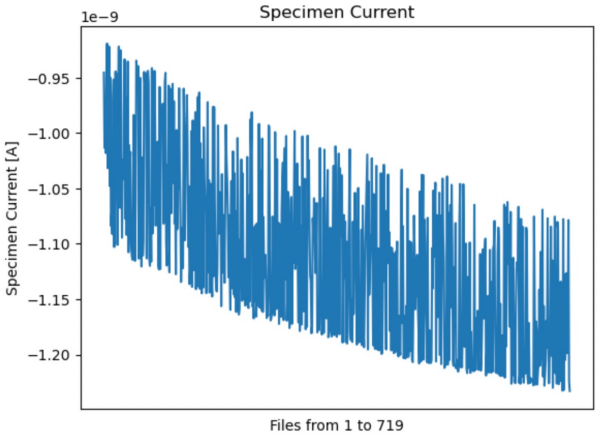
Visualizing Metadata

- Visualizing the evolution of chamber pressure values during the experiment
- Chamber pressure affects milling accuracy
- Expected to decrease over the course of the experiment



Visualizing Metadata

- Visualizing the changes of specimen current values during the experiment
- Specimen current affects the brightness of the SEM image and Energy-Dispersive X-ray Spectroscopy (EDS) signal



Conclusions

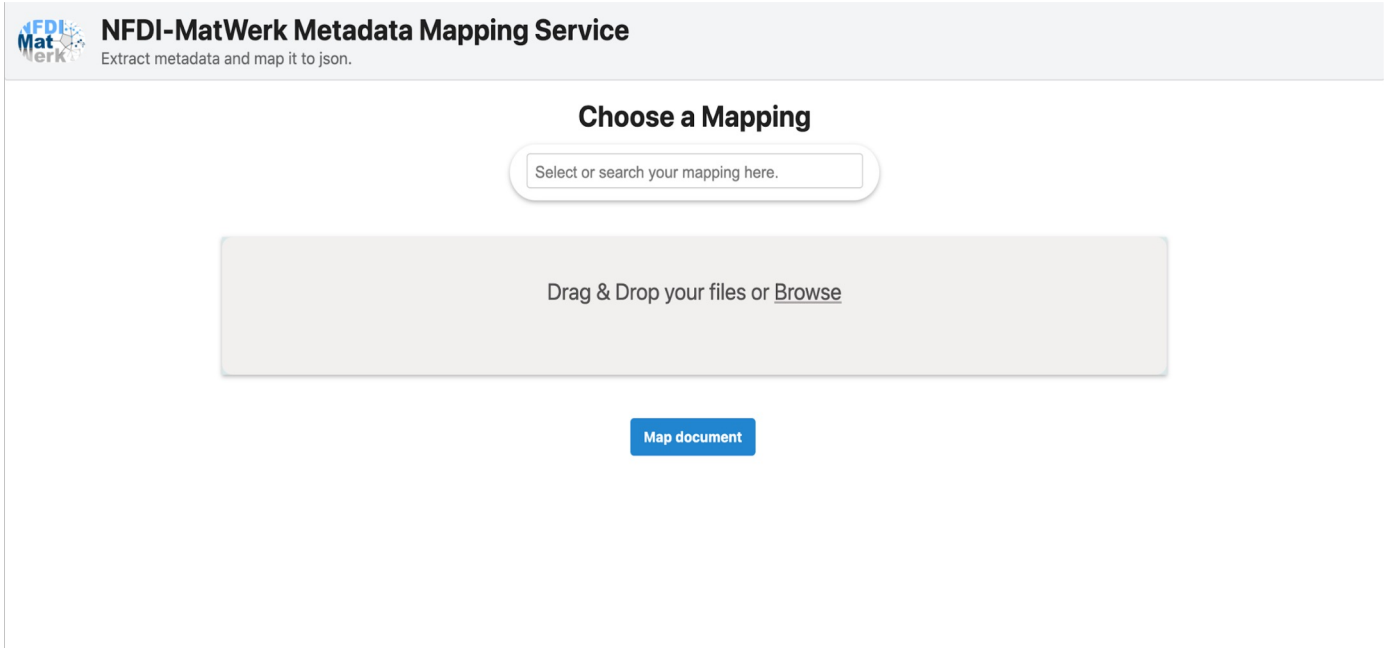
- The Visual Analyzer:
  - allows for a quick overview of the experiment as a whole
  - facilitates the comparison of experiment results
  - automates and optimizes the analysis of metadata, expediting the decision-making process
- It can be expanded and adapted according to the needs of the scientists
- Open source:
  - https://bwsyncandshare.kit.edu/s/nemrjdMGKnLfmt2

Q & A

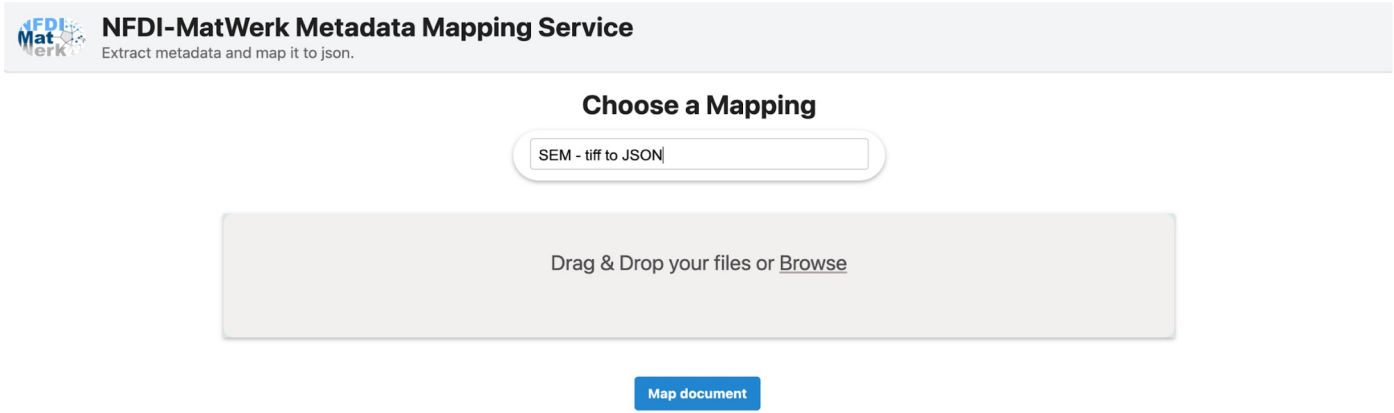
Thank You

Back-up

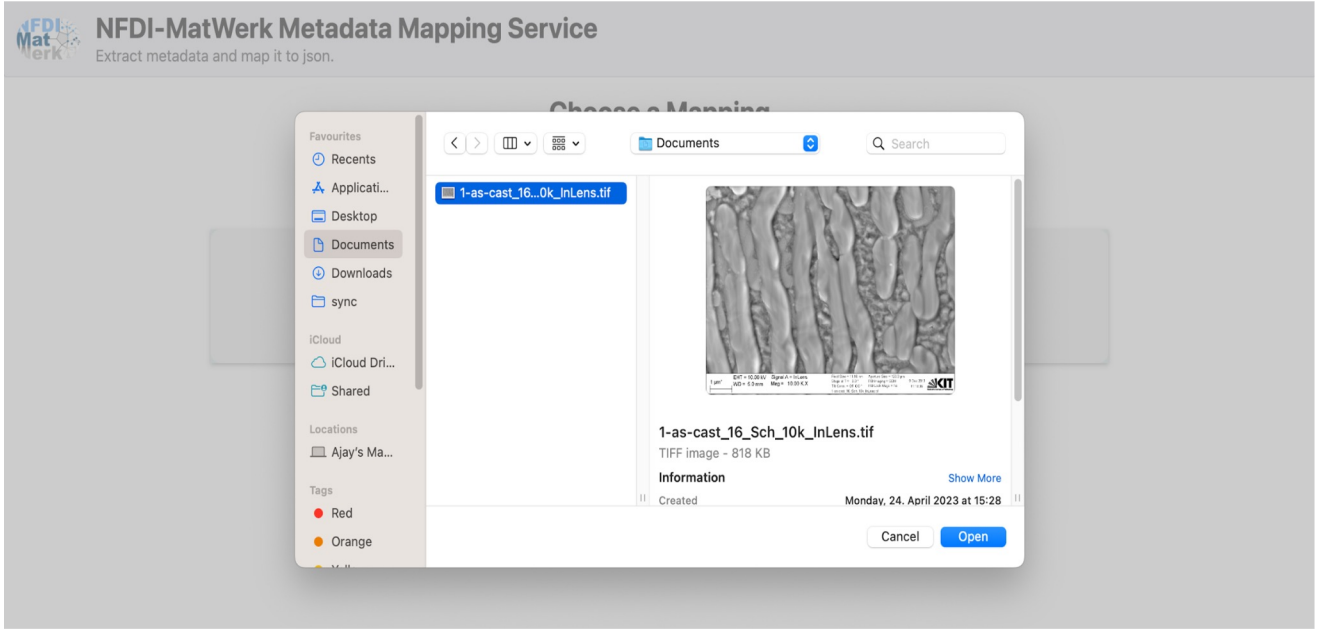
Interface for Mapping Service



Interface for Mapping Service



Interface for Mapping Service



Interface for Mapping Service