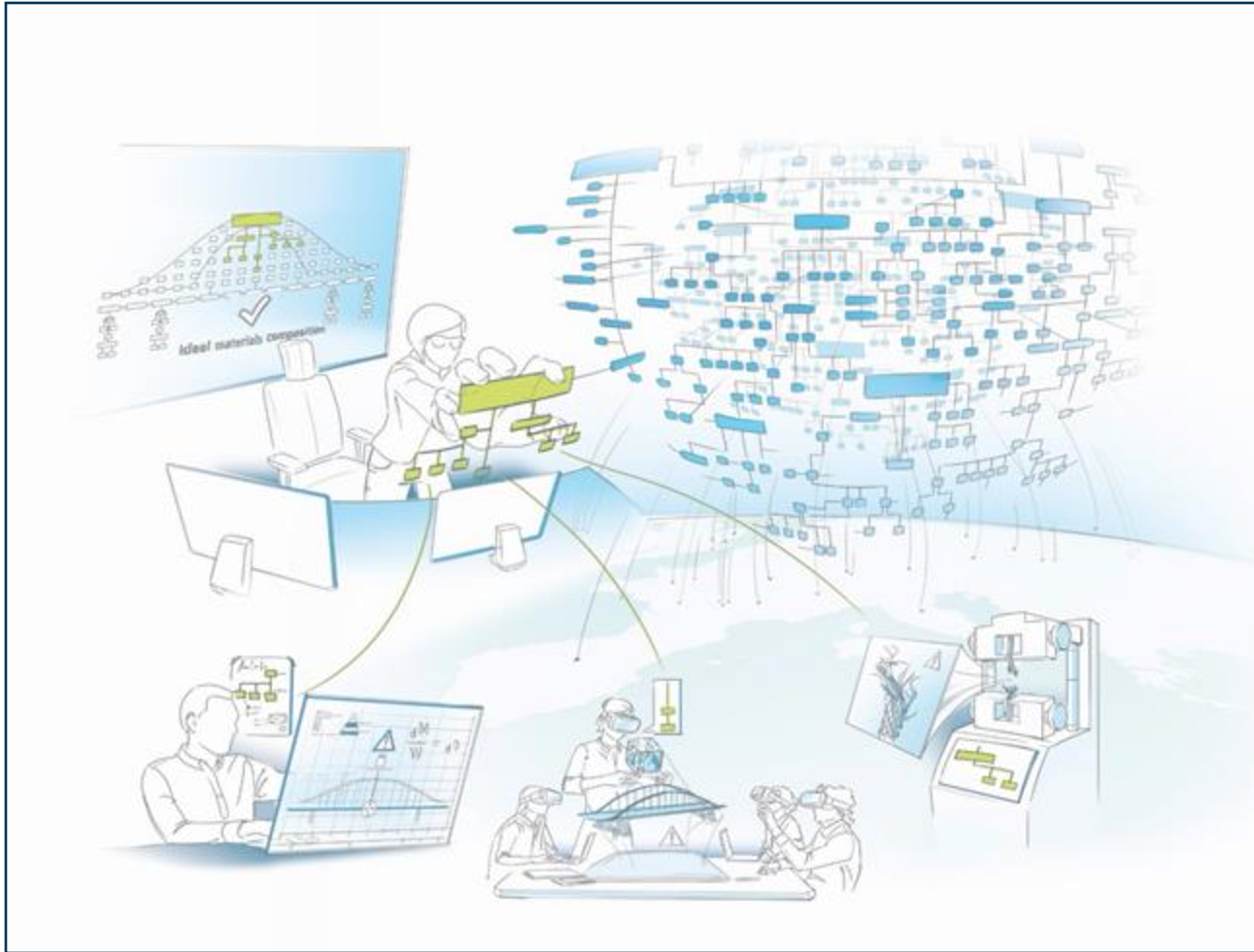
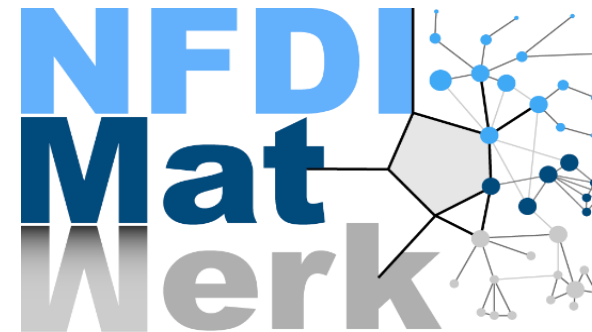


Metadata Management in practice using MatWerk tools

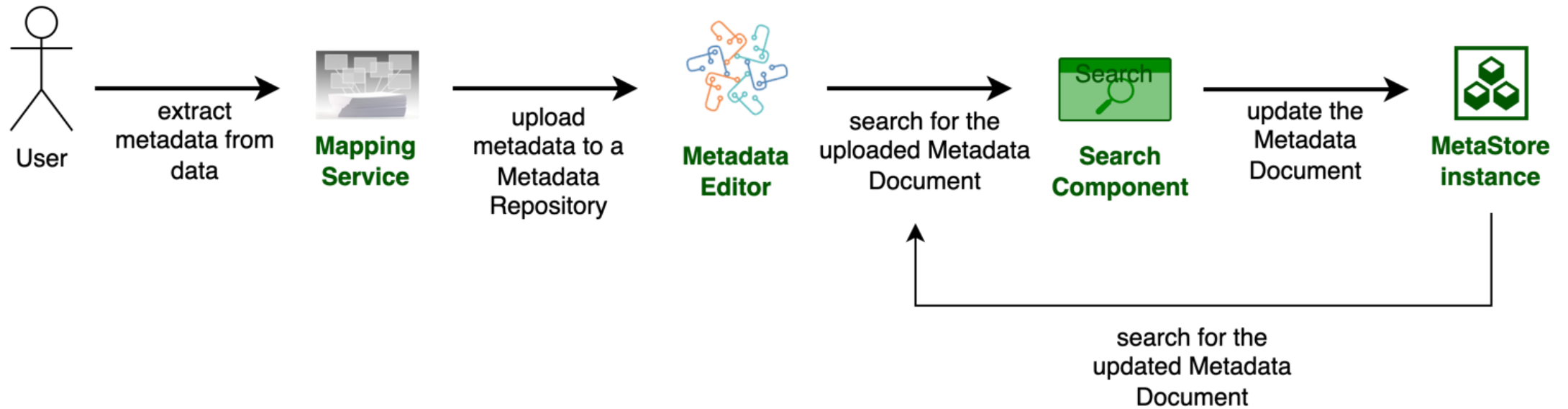


Sabrine Chelbi
Scientific Computing Center (SCC)
Karlsruhe Institute of Technology (KIT)

NATIONAL RESEARCH DATA
INFRASTRUCTURE FOR
MATERIALS SCIENCE &
ENGINEERING



Use Case



NFDI-MatWerk Dashboard



- Collection of web front-end services for NFDI-MatWerk available under this link:
<https://t1p.de/frontend-dashboard>



NFDI-MatWerk Dashboard

This collection of web front-ends provides easy access to the RESTful services of a MatWerk instance run by the DEM department at SCC.

A Documentation for the MatWerk instance can be found [here](#)



NFDI-MatWerk Metadata Repository UI

Manage and access your metadata schemas and documents on the MatWerk instance.



NFDI-MatWerk Data Repository UI

Manage and access your research data described by DataCite metadata on the MatWerk instance.



Mapping Service

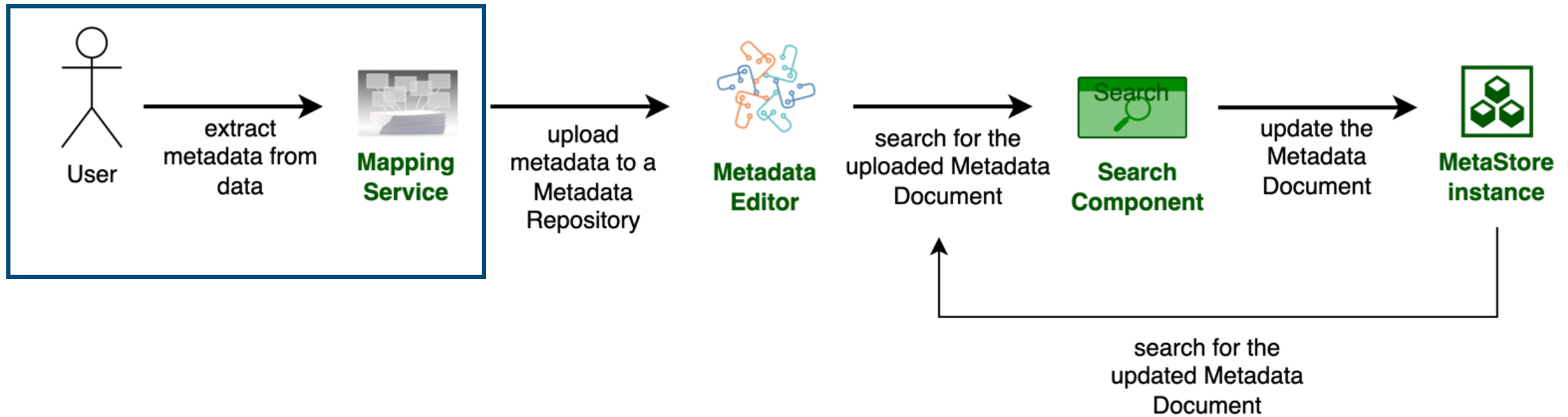
View Mapping Service interface.



SKOSMOS Service

SKOSMOS instance for MatWerk published controlled vocabularies.

Use Case



Introduction to the Mapping Service

- Extraction of metadata from different data files.
- Mapping of this metadata to published metadata schemas.
- Available Mappings:
 - Thermofischer SEM TIFF to JSON
 - MRI to JSON
 - Zeiss SEM to JSON
 - APE-HE NeXus to JSON

NFDI-MatWerk Dashboard

This collection of web front-ends provides easy access to the RESTful services of a MatWerk instance run by the DEM



Mapping Service UI

Extract metadata and map it to json.

The Mapping Service is a tool designed to extract metadata from different data-files, and map this metadata to published metadata schemas. [Show More](#)

Choose a suitable mapping from available options

Thermofisher SEM TIFF to JSON

This plugin is able to handle a variety of SEM images generated by Thermofisher/FEI instruments and extract and map their metadata to the SEM schema. A resulting metadata document in JSON format is then created. LU: 30.11.2023

Select

MRI to JSON

Takes a single .dcm or zipped directory of .dcm files and maps to the MRI schema returning a JSON metadata document. LU: 01.02.2024

Select

Zeiss SEM to JSON

This plugin is able to handle a variety of SEM images and processes them using the Hyperspy library. A resulting metadata document in JSON format is then created. LU: 15.02.2024

Select

APE-HE NeXus to JSON

This plugin allows the creation of a JSON document containing metadata extracted from Nexus files generated by Advanced Photoelectric Effect - High Energy experiments. Last Updated: 27.11.2024

Select

Please select a mapping from the list above.

Drag & Drop your files or [Browse](#)
(File size is limited to 5MB)

Execute Mapping

SKOSMOS Service

SKOSMOS instance for MatWerk published controlled vocabularies.

- Task: extract metadata from an existing SEM (Scanning Electron Microscopy) image.
- Tutorial: <https://t1p.de/matwerk-tutorial>
- SEM images: https://t1p.de/sem_images



Mapping Service UI

Extract metadata and map it to json.

The Mapping Service is a tool designed to extract metadata from different data-files, and map this metadata to published metadata schemas. [Show More](#)

Choose a suitable mapping from available options

Thermofisher SEM TIFF to JSON

This plugin is able to handle a variety of SEM images generated by Thermofisher/FEI instruments and extract and map their metadata to the SEM schema. A resulting metadata document in JSON format is then created. LU: 30.11.2023

Select

MRI to JSON

Takes a single .dcm or zipped directory of .dcm files and maps to the MRI schema returning a JSON metadata document. LU: 01.02.2024

Select

Zeiss SEM to JSON

This plugin is able to handle a variety of SEM images and processes them using the Hyperspy library. A resulting metadata document in JSON format is then created. LU: 15.02.2024

Select

APE-HE NeXus to JSON

This plugin allows the creation of a JSON document containing metadata extracted from Nexus files generated by Advanced Photoelectric Effect - High Energy experiments. Last Updated: 27.11.2024

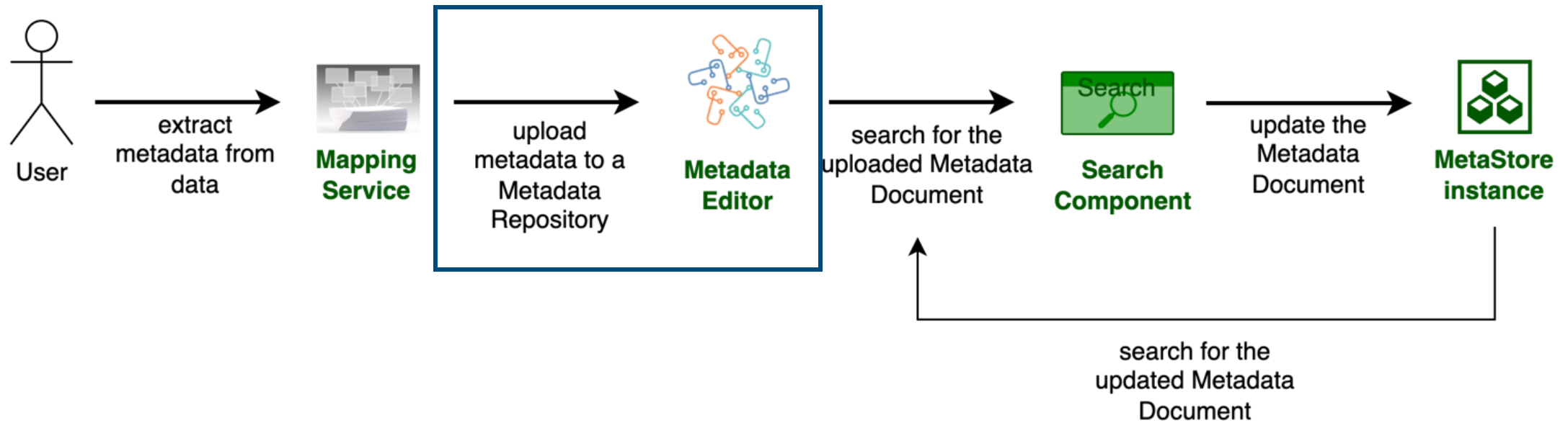
Select

Please select a mapping from the list above.

Drag & Drop your files or Browse
(File size is limited to 5MB)

Execute Mapping

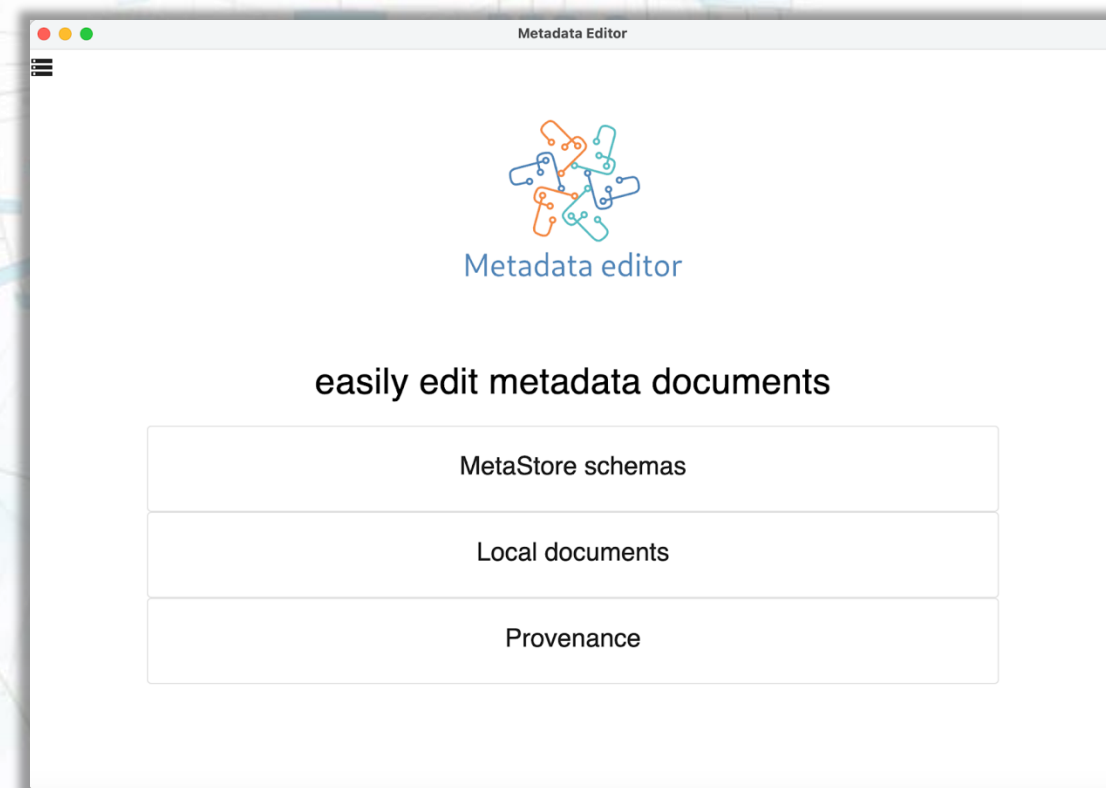
Use Case



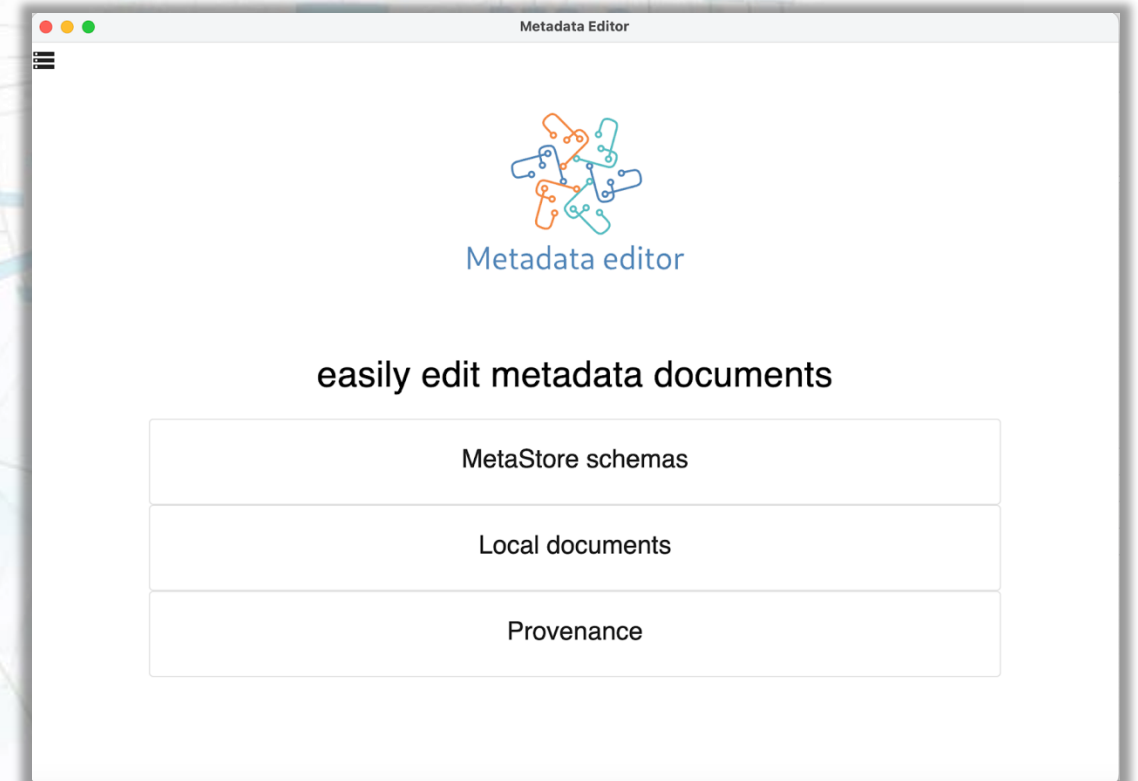
Metadata Editor

- Desktop application developed and maintained by eXact lab as part of the NFFA-Europe Pilot project
- User interface to support users while ingesting and editing their metadata documents
- Two different metadata repository instances:
 - MetaRepo
 - NFDI-MatWerk Repository

Metadata

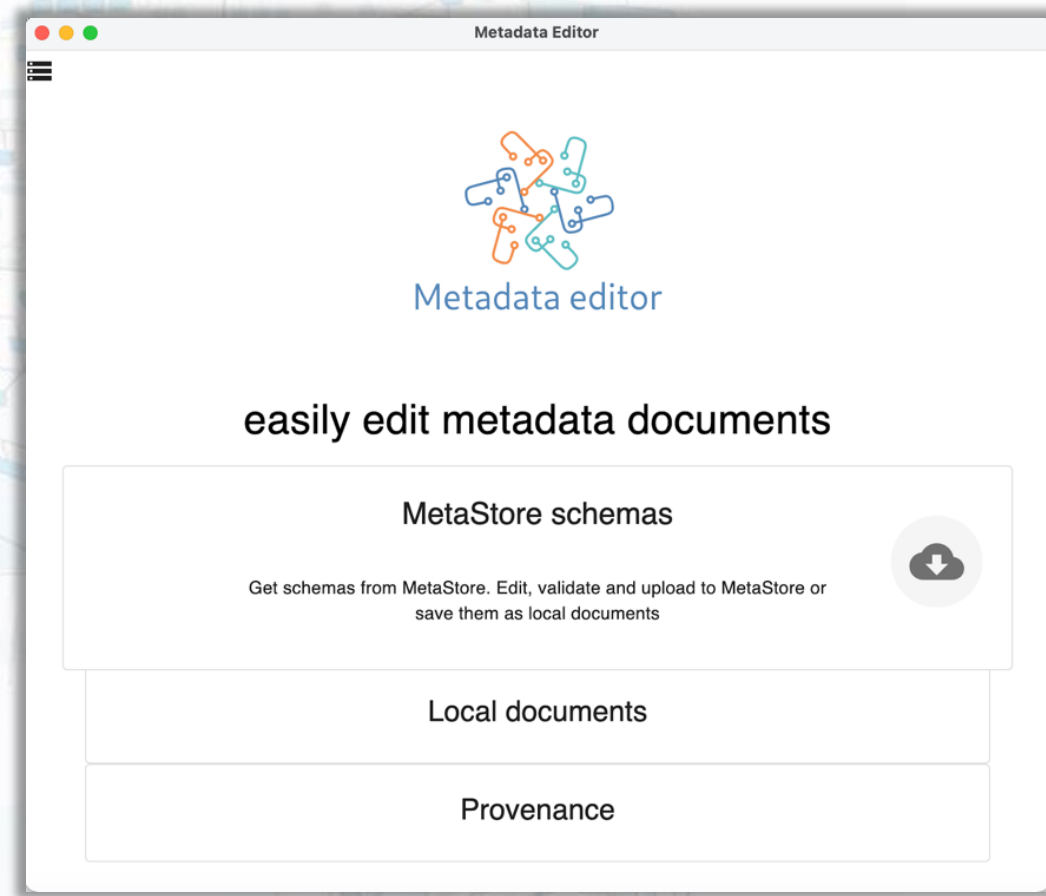


- Main functionalities
 - Get Schema Templates, Manage Metadata Documents
 - Load and manage Metadata Documents
 - Get document provenance



Metadata Editor: Get Schema Templates/Manage Metadata Documents

- Retrieve registered schemas from the MetaStore instance using the first box “MetaStore schemas”



Metadata Editor: Get Schema Templates/Manage Metadata Documents

- Registered schemas are grouped using:
 - thematic “label” tags: group schemas which have common characteristics because they belong to the same part of the workflow.
 - Schema identifier
 - Optionally version number
- Fill out the form manually or load an existing filled-in metadata document.

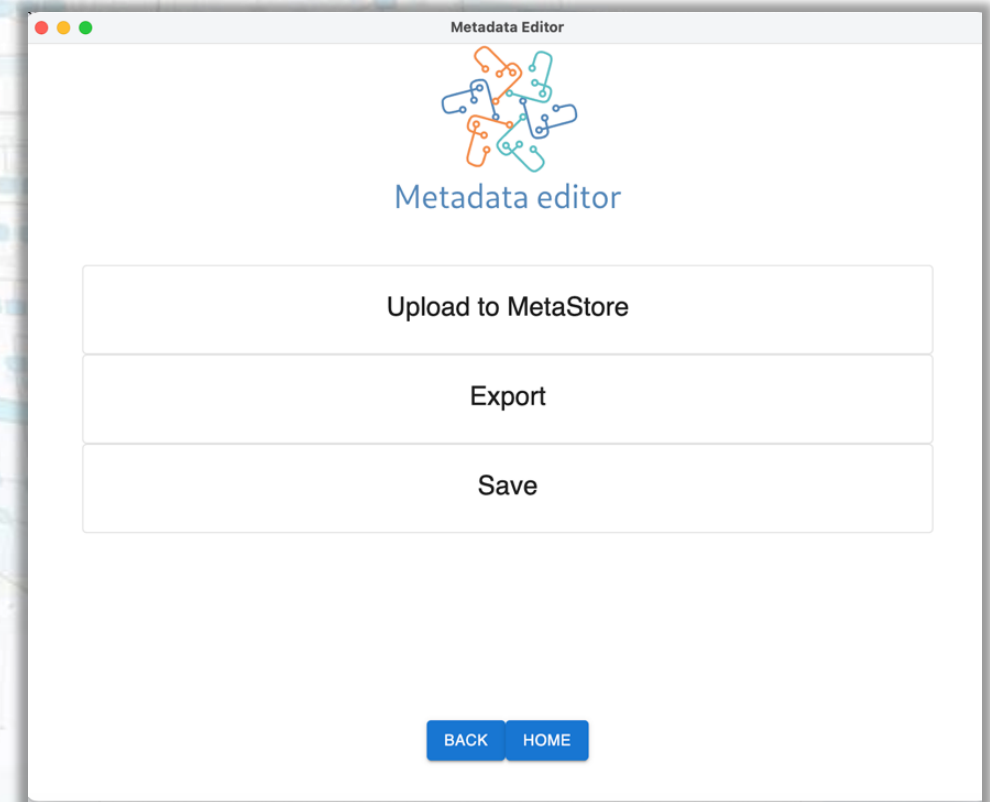
The screenshot shows the 'Metadata Editor' web application. At the top, there are three dropdown menus: 'Label' (set to 'raw data'), 'Schema ID' (set to 'scanning-electron-microscopy'), and 'Version' (set to '7'). Below these are two blue buttons: 'LOAD SCHEMA' and 'LOAD JSON DOCUMENT'. A lock icon and the word 'Entry' are centered below the buttons. The main form area contains several fields: 'Technique*' (text input), 'Measurement Purpose*' (dropdown), 'Measurement Description' (text input), 'Equipment' (text input), 'Consumables' (text input with a '+' icon and a detailed description: '(Optional) - Auxiliary entity used during Fabrication, Sample Preparation or Measurement which has a limited time capacity or is limited in its number of uses before it is disposed of, necessary to the process itself and normally bought from third party manufacturers. Examples are: gloves, syringes, wipes, etching solutions, glass slides, spatulas, weighing paper, two-sided tape.'), 'Parents*' (text input with a '+' icon and 'No Selection' below it), 'Entry ID' (dropdown menu with 'No data' selected), 'Title*' (text input), 'Start Time' (text input), 'End Time*' (text input), 'Program' (dropdown), 'Revision' (dropdown), 'User' (dropdown), and 'Instrument' (dropdown). At the bottom, there are three blue buttons: 'BACK', 'HOME', and 'DONE'.

- As a next step, the user has 3 options:
 - Upload the document to the MetaStore instance
 - Export the document as a JSON file
 - Save it locally as a JME file

The screenshot shows the Metadata Editor web application. At the top, there's a header with the NFDI Mat Werk logo and the text 'Metadata Editor'. Below the header, there's a navigation bar with a hamburger menu icon and the text 'LOGOUT (SABRINECHELBI)'. The main content area features the NFDI Mat Werk logo and the text 'Metadata editor'. Below this, there's a form titled 'Metadata record'. The form has a dropdown menu labeled 'Related Resource Id Type' with 'URL' selected. Below the dropdown is a text input field labeled 'Related resource identifier' containing the URL 'https://t1p.de/Zeiss_SEM_30'. At the bottom of the form, there are three buttons: 'UPLOAD', 'BACK', and 'HOME'.

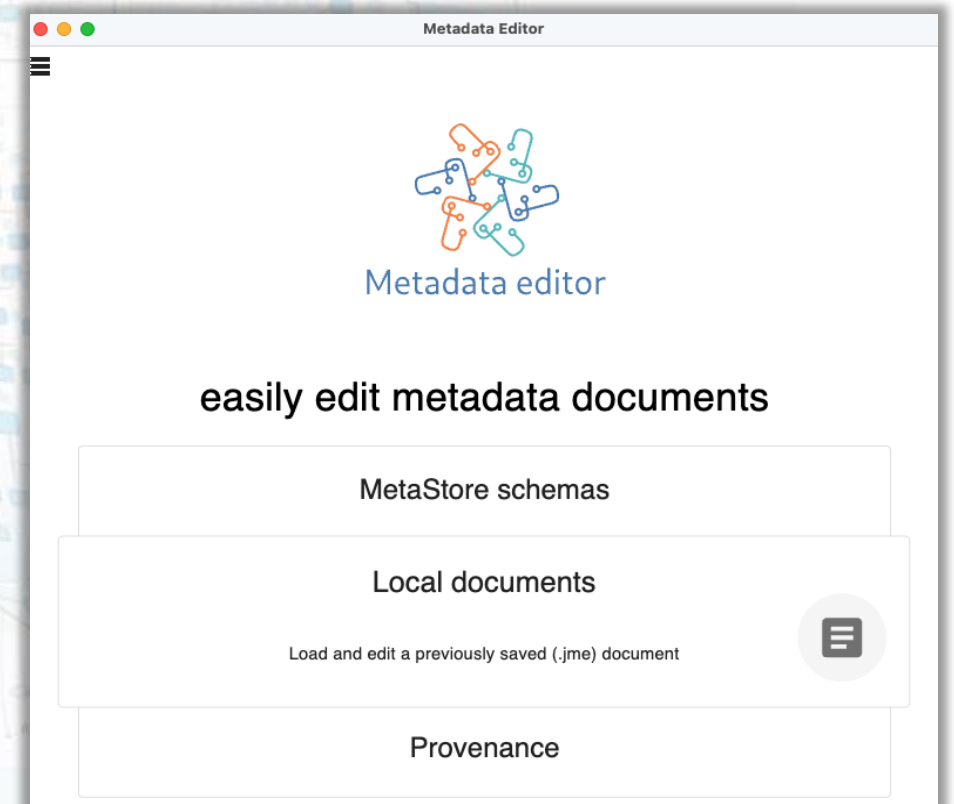
Metadata Editor: Get Schema Templates/Manage Metadata Documents

- As a next step, the user has 3 options:
 - Upload the document to the MetaStore instance
 - Export the document as a JSON file
 - Save it locally as a JME file



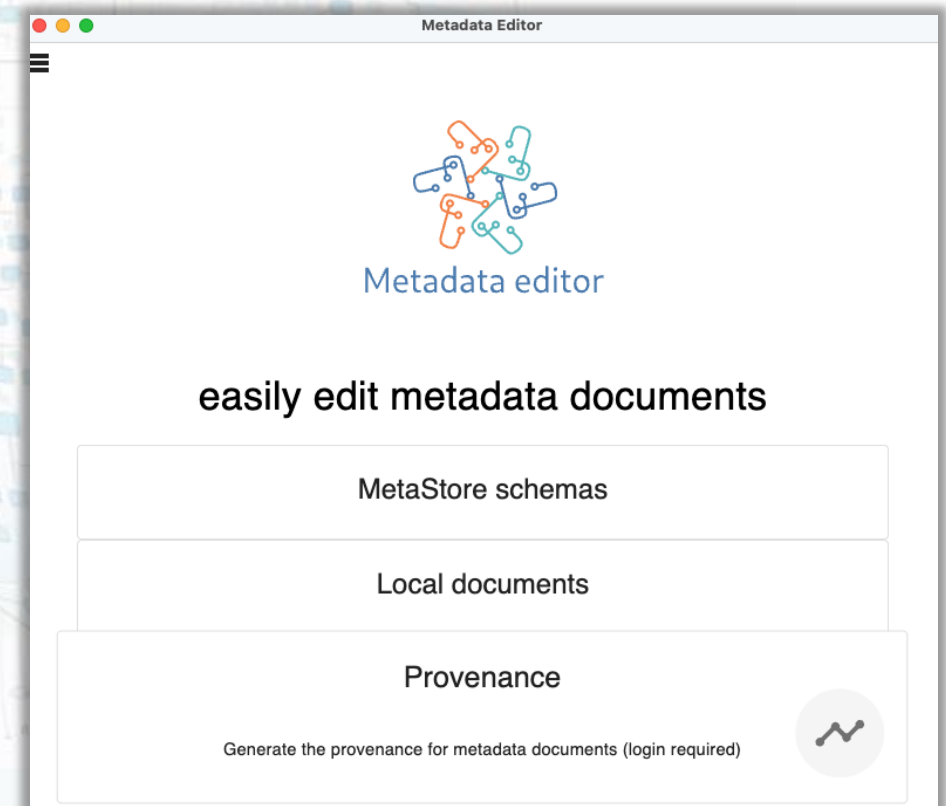
Metadata Editor: Load and Manage Metadata Documents

- Further editing of the previously saved JME document.
- The editing and saving of the document follows the same process.

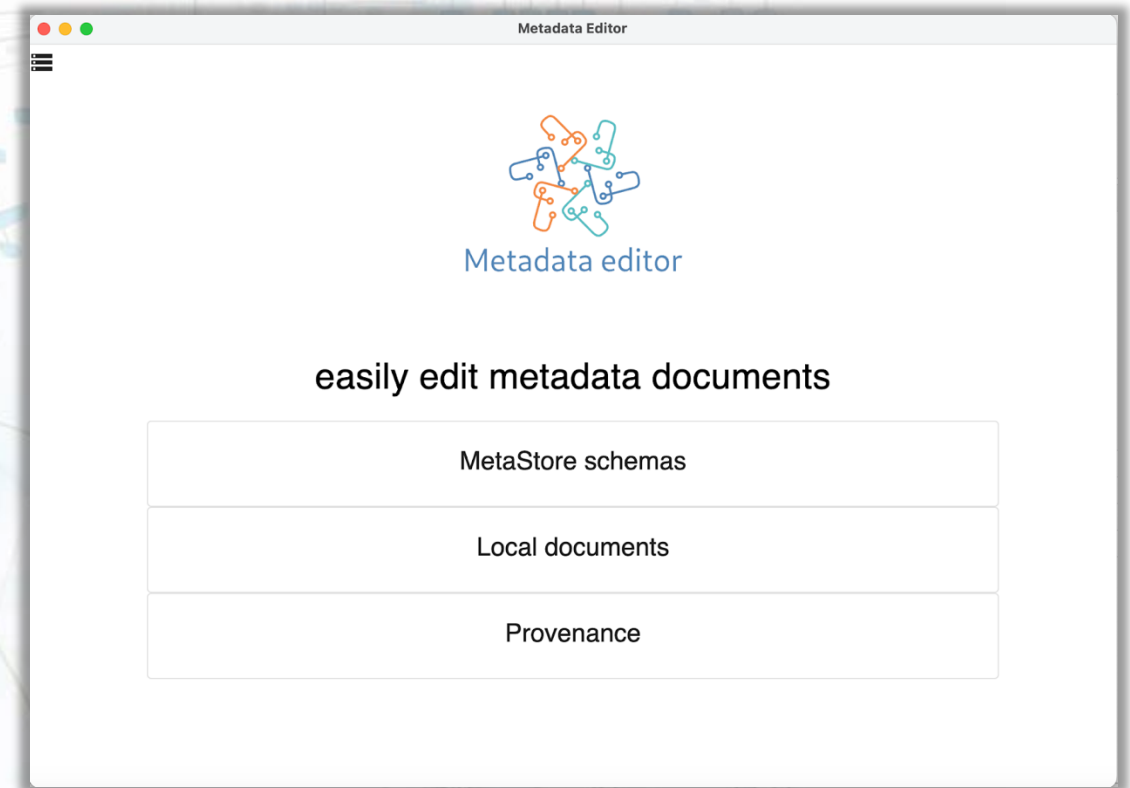


Metadata Editor: Get document provenance

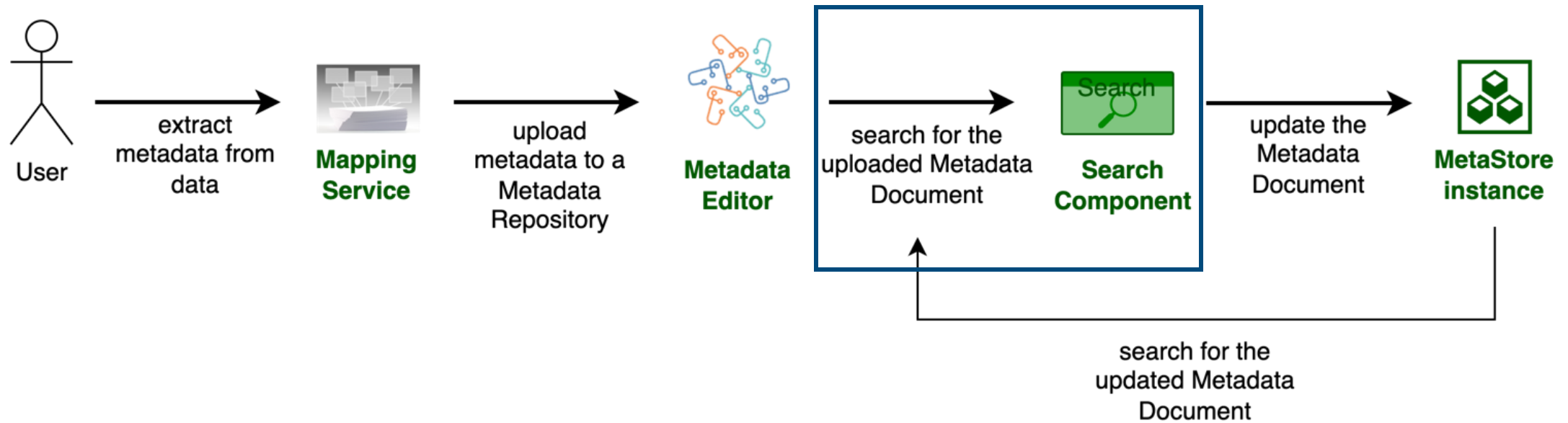
- The provenance is tracked backwards and is retrieved by iteratively keeping track of the “Parent” field inside the other registered metadata documents, If available.
- Required information: schema identifier, the corresponding metadata document.
- The provenance JSON file will be automatically generated and can be saved locally.
- In case the metadata document does not include a “Parent” field, an error will be displayed.



- Task: upload your metadata document to a Metadata Repository.



Use Case



Search Component

- Aim: find relevant data by performing a search based on metadata.
- Only publicly available metadata documents are listed.
- Filtering is available.
- After the login, users can see their documents.
- <https://t1p.de/search-component>

NFDI4MatWerk Metadata Search

Search

Clear 0 Filters

SORT BY
Relevance

INDEX

- ☐ metastore-user_description 18
- ☐ metastore-scanning-electron-microscopy 6
- ☐ metastore-sem 1

PROGRAM VERSION

- ☐ V05.07.00.00 : 08-Jul-14 4
- ☐ 14.5.1.432 1
- ☐ 3.8.9.194.3 1
- ☐ V06.00.00.00 : 09-Jun-16 1

USERNAME

- ☐ SABINE 3
- ☐ USER 2
- ☐ user 2

STAGE ALIGNMENT DONE

- ☐ 1 5

ACCELERATION VOLTAGE

- ☐ 0-5 2
- ☐ 6-10 2
- ☐ 11-15 0
- ☐ 16-20 1
- ☐ >20 3

END TIME

- ☐ This Year 0
- ☐ Last Year 0
- ☐ 2 years ago 1
- ☐ Older 6

ROLE

- ☐ Data Curator 7
- ☐ Team Member 6
- ☐ Instrument Scientist 3
- ☐ Team Leader 2

Showing 1 - 13 out of 13

SEM : 20000 KV

Unknown SEM Device

sample SEM image Thermo Fisher Helios

HeliosPFIB

feasibility (quick check, rough estimate)

User user

Show Metadata Record

SEM : 10000 KV

Unknown SEM Device

sample SEM image FEI Helios Nanolab600

Unspecified Title

feasibility (quick check, rough estimate)

User user

Show Metadata Record

SEM : 10 KV :: StageAligned

Unknown SEM Device

1-as-cast_16_Sch_10k_InLens.tif

Auriga 60 (Auriga 60-46-18)

No purpose provided.

User SABINE

Show Metadata Record

SEM : 20 KV :: StageAligned

Unknown SEM Device

SCE05_17.tif

Zeiss Auriga (Auriga 60-46-18)

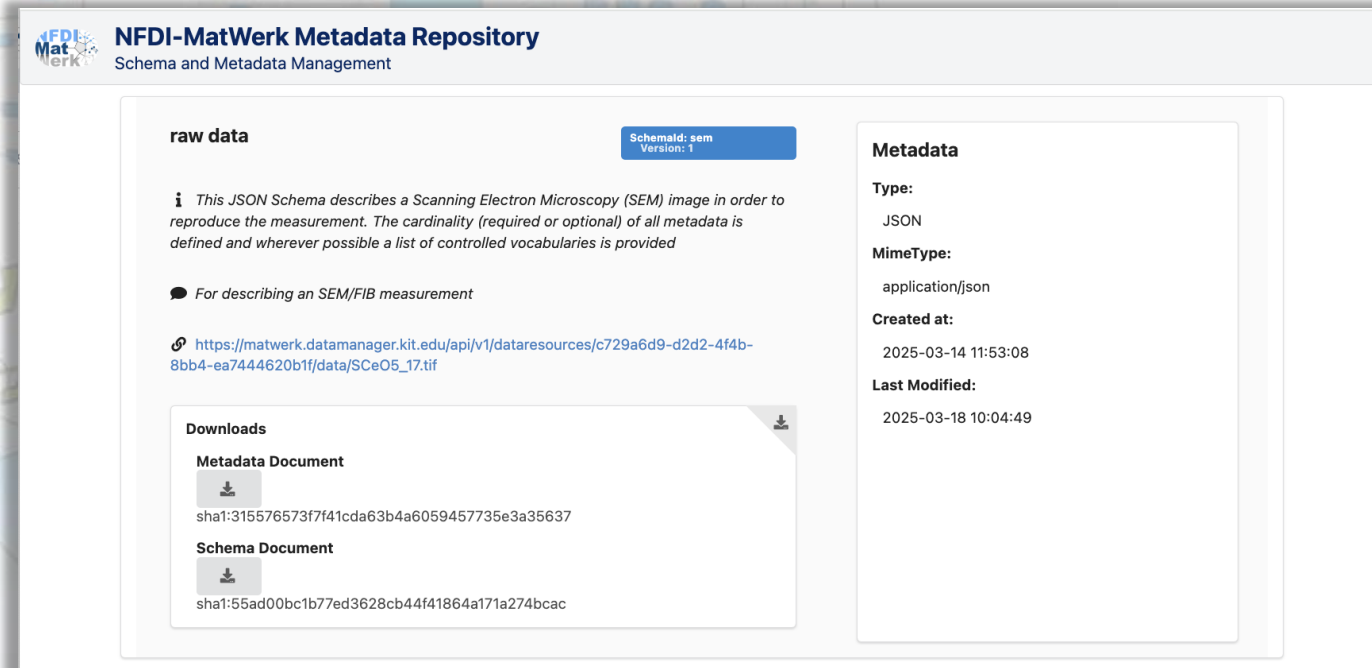
completeness check (presence or absence of given properties)

User SABINE

Show Metadata Record

Search Component: Landing Page

- Different information are provided: schema identifier, label, type of the document,...
- Metadata documents are available only when they are public.
 - The user won't benefit from the advantages of the FAIR principles (not findable, not reusable)
 - The right permissions should be changed and a license should be added.



The screenshot displays the 'NFDI-MatWerk Metadata Repository' interface. At the top, the title 'NFDI-MatWerk Metadata Repository' is followed by the subtitle 'Schema and Metadata Management'. The main content area is divided into two primary sections: 'raw data' on the left and 'Metadata' on the right. The 'raw data' section includes a blue button labeled 'SchemaId: sem Version: 1', an information icon with a descriptive paragraph about the JSON schema for SEM images, a speech bubble icon with a note about SEM/FIB measurements, and a link to a specific data resource. Below this is a 'Downloads' box containing two items: a 'Metadata Document' with a download icon and a SHA1 hash, and a 'Schema Document' with a download icon and a SHA1 hash. The 'Metadata' section on the right lists the document's 'Type' as JSON, 'MimeType' as application/json, 'Created at' timestamp as 2025-03-14 11:53:08, and 'Last Modified' timestamp as 2025-03-18 10:04:49.

NFDI-MatWerk Metadata Repository
Schema and Metadata Management

raw data SchemaId: sem Version: 1

i This JSON Schema describes a Scanning Electron Microscopy (SEM) image in order to reproduce the measurement. The cardinality (required or optional) of all metadata is defined and wherever possible a list of controlled vocabularies is provided

• For describing an SEM/FIB measurement

https://matwerk.datamanager.kit.edu/api/v1/dataresources/c729a6d9-d2d2-4f4b-8bb4-ea7444620b1f/data/SCeO5_17.tif

Downloads

Metadata Document
Download icon
sha1:315576573f7f41cda63b4a6059457735e3a35637

Schema Document
Download icon
sha1:55ad00bc1b77ed3628cb44f41864a171a274bcac

Metadata

Type:
JSON

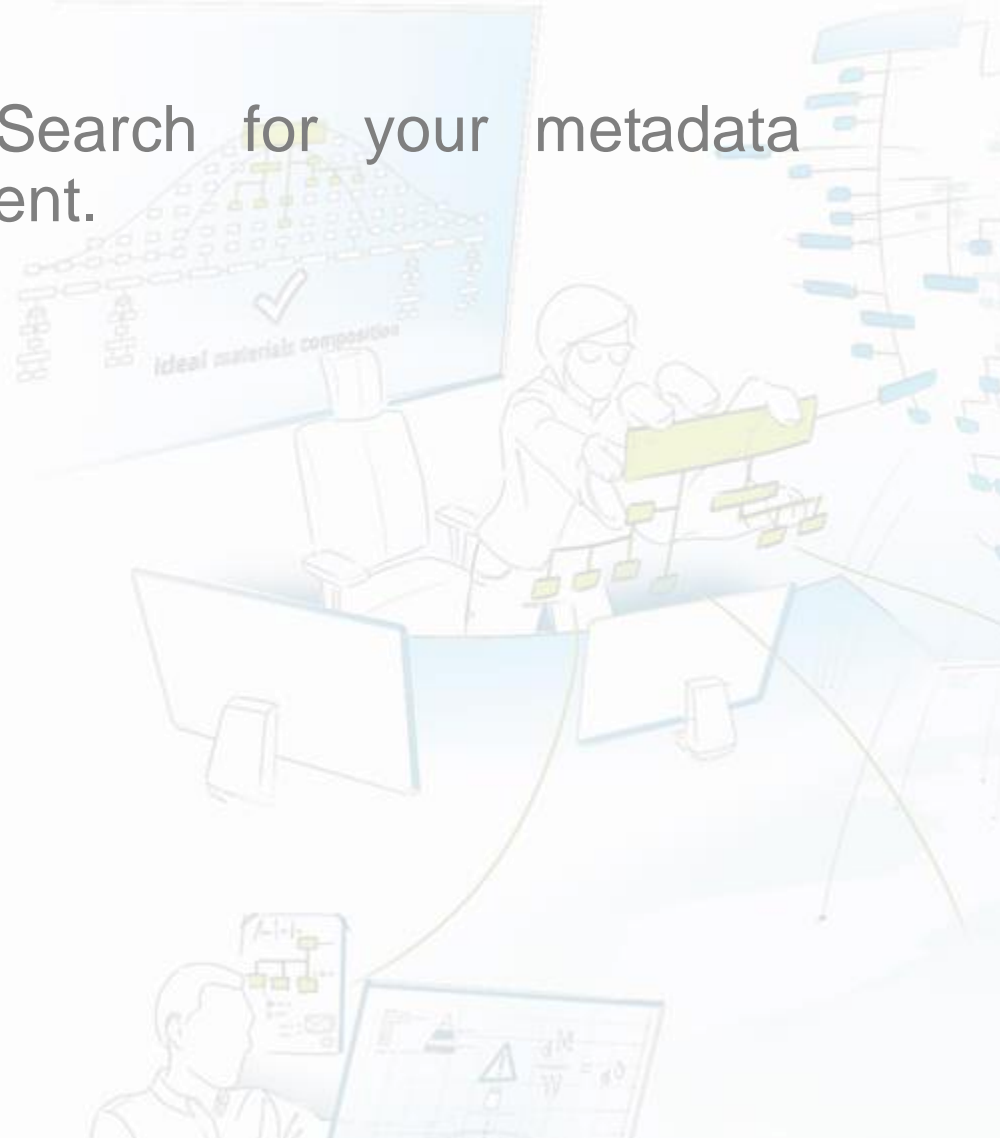
MimeType:
application/json

Created at:
2025-03-14 11:53:08

Last Modified:
2025-03-18 10:04:49

Hands-on

- Task: Search for your metadata document.



NFDI4MatWerk Metadata Search

Search

Clear 0 Filters

SORT BY
Relevance

INDEX

- ☐ metastore-user_description 18
- ☐ metastore-scanning-electron-microscopy 4
- ☐ metastore-sem 1

PROGRAM VERSION

- ☐ V05.07.00.00 : 08-Jul-14 2
- ☐ 14.5.1.432 1
- ☐ 3.8.9.1943 1
- ☐ V06.00.00.00 : 09-Jun-16 1

USERNAME

- ☐ SABINE 3
- ☐ user 2

STAGE ALIGNMENT DONE

- ☐ 1 3

ACCELERATION VOLTAGE

- ☐ 0-5 0
- ☐ 6-10 2
- ☐ 11-15 0
- ☐ 16-20 1
- ☐ >20 3

END TIME

- ☐ This Year 0
- ☐ Last Year 0
- ☐ 2 years ago 1
- ☐ Older 4

ROLE

- ☐ Data Curator 7
- ☐ Team Member 6
- ☐ Instrument Scientist 3
- ☐ Team Leader 2

Showing 1 - 13 out of 13

SEM 20000 kV

Unknown SEM Device

sample SEM image Thermo Fisher Helios

HeliosPFIB

feasibility (quick check, rough estimate)

User user

Show Metadata Record

SEM 10000 kV

Unknown SEM Device

sample SEM image FEI Helios Nanolab600

Unspecified Title

feasibility (quick check, rough estimate)

User user

Show Metadata Record

SEM 10 kV StageAligned

Unknown SEM Device

1-as-cast_16_Sch_10k_InLens.tif

Auriga 60 (Auriga 60-46-18)

No purpose provided.

User SABINE

Show Metadata Record

SEM 20 kV StageAligned

SCe05_17.tif

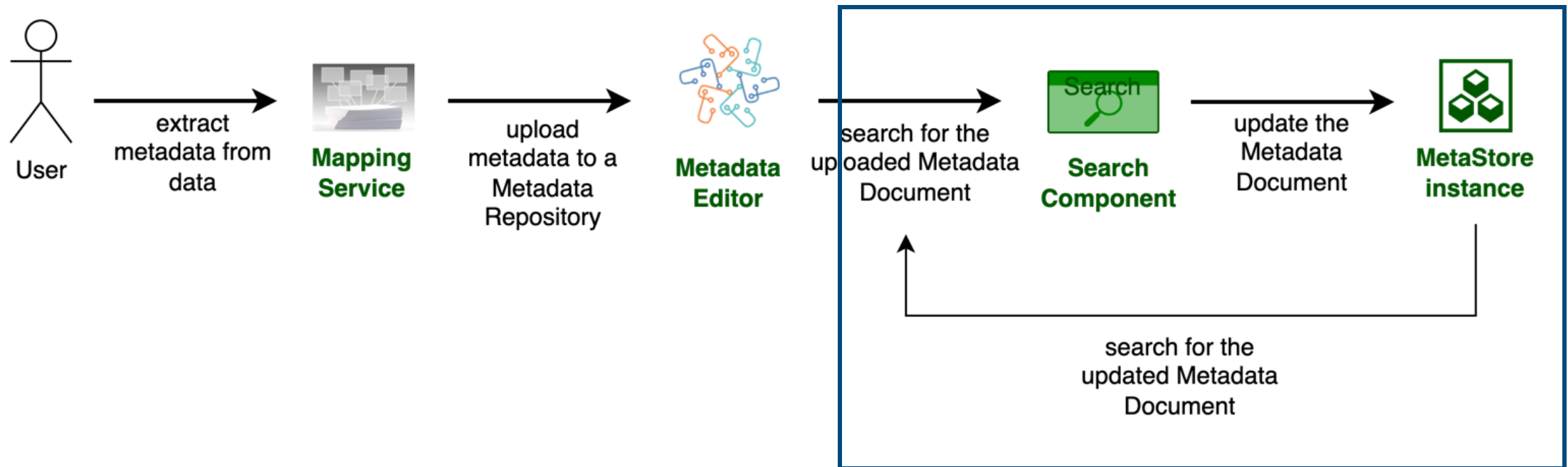
Zeiss Auriga (Auriga 60-46-18)

completeness check (presence or absence of given properties)

User SABINE

Show Metadata Record

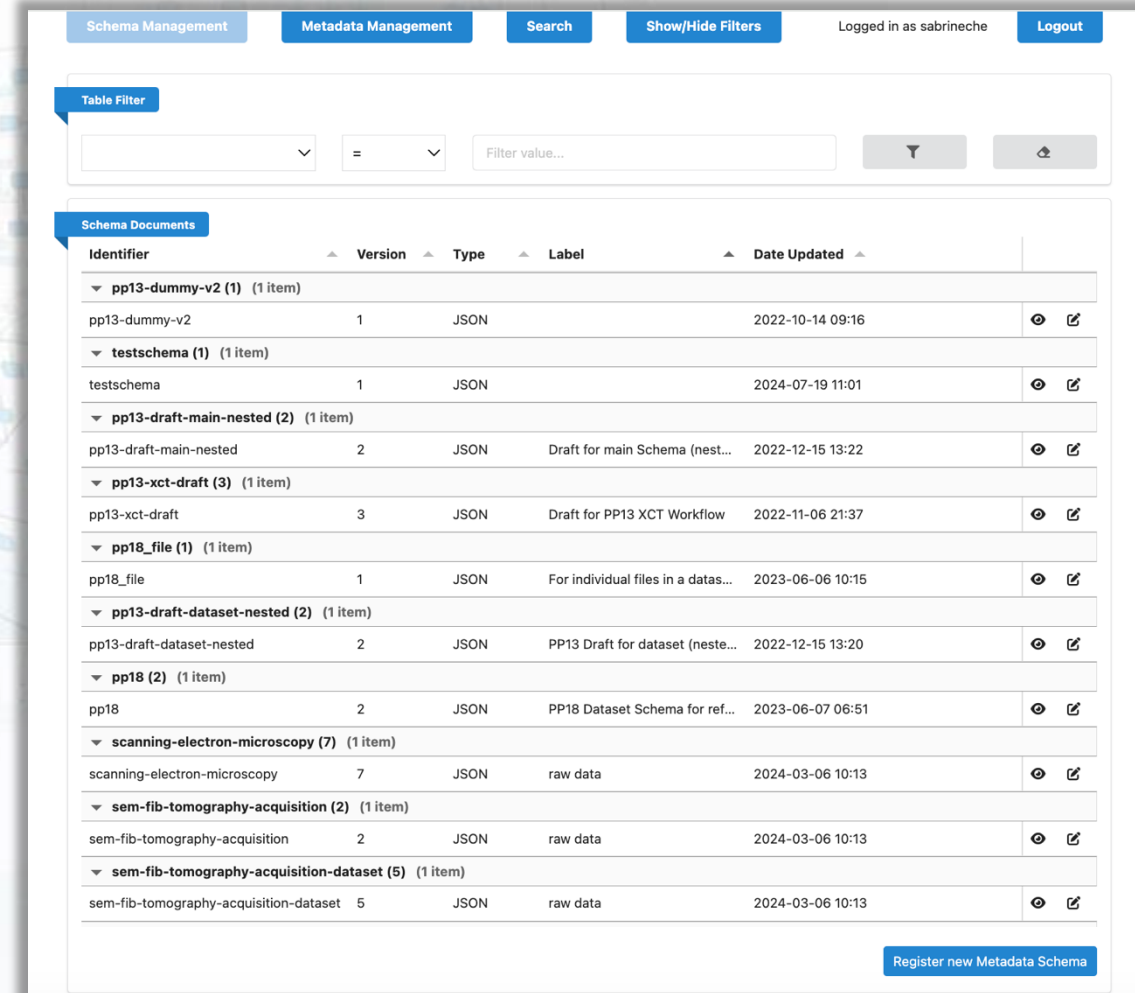
Use Case



- Developed within DEM at SCC-KIT.
- Metadata repository framework for storing schemas and metadata documents and supports both formats XML and JSON.
- It allows to:
 - register and later update XML/JSON schemas
 - add metadata documents written according to a registered schema and later update them
 - validate metadata against a registered schema
- All functionalities are described with the help of a clear and intuitive REST-API Structure.
- NFDI-MatWerk Metadata Repository is a MetaStore instance for the NFDI-MatWerk project.

GET	/api/v1/schemas/{schemaId}	Get schema record by schema id (and version).
GET	/api/v1/schemas	Get all schema records.
PUT	/api/v1/schemas/{schemaId}	Update a schema record.
POST	/api/v1/schemas	Register a schema document and its record.
POST	/api/v1/schemas/{schemaId}/validate	Validate a metadata document.
DELETE	/api/v1/schemas/{schemaId}	Delete a schema record.
GET	/api/v1/metadata/{id}	Get a metadata record by id.
GET	/api/v1/metadata	Get all records.
PUT	/api/v1/metadata/{id}	Update a metadata record and/or metadata document.

- Registered schemas are publicly available in read-only mode.
- Schemas are listed in a table with different column headers: “identifier”, “Version”, “Type”, “Label” and “Date Updated”.
- Filtering is also available based on “schema identifier”, “Type” or “label”.
- Schema records:
 - include the metadata information of a schema
 - They can be read and updated using the icons on the right side.
 - Schema itself can be also read and updated.



The screenshot displays the 'Schema Management' section of the NFDI-MatWerk Metadata Repository. The interface includes a navigation bar with tabs for 'Schema Management', 'Metadata Management', 'Search', and 'Show/Hide Filters'. The user is logged in as 'sabrineche' and can click 'Logout'. Below the navigation bar is a 'Table Filter' section with a dropdown menu, an equals sign, another dropdown, and a text input field for 'Filter value...'. The main content area, titled 'Schema Documents', contains a table with columns: Identifier, Version, Type, Label, and Date Updated. The table lists various schemas, each with a collapse/expand icon, a list of items, and a 'Read' (eye icon) and 'Update' (pencil icon) button. At the bottom right, there is a button labeled 'Register new Metadata Schema'.

Identifier	Version	Type	Label	Date Updated
▼ pp13-dummy-v2 (1) (1 item)				
pp13-dummy-v2	1	JSON		2022-10-14 09:16
▼ testschema (1) (1 item)				
testschema	1	JSON		2024-07-19 11:01
▼ pp13-draft-main-nested (2) (1 item)				
pp13-draft-main-nested	2	JSON	Draft for main Schema (nest...	2022-12-15 13:22
▼ pp13-xct-draft (3) (1 item)				
pp13-xct-draft	3	JSON	Draft for PP13 XCT Workflow	2022-11-06 21:37
▼ pp18_file (1) (1 item)				
pp18_file	1	JSON	For individual files in a datas...	2023-06-06 10:15
▼ pp13-draft-dataset-nested (2) (1 item)				
pp13-draft-dataset-nested	2	JSON	PP13 Draft for dataset (neste...	2022-12-15 13:20
▼ pp18 (2) (1 item)				
pp18	2	JSON	PP18 Dataset Schema for ref...	2023-06-07 06:51
▼ scanning-electron-microscopy (7) (1 item)				
scanning-electron-microscopy	7	JSON	raw data	2024-03-06 10:13
▼ sem-fib-tomography-acquisition (2) (1 item)				
sem-fib-tomography-acquisition	2	JSON	raw data	2024-03-06 10:13
▼ sem-fib-tomography-acquisition-dataset (5) (1 item)				
sem-fib-tomography-acquisition-dataset	5	JSON	raw data	2024-03-06 10:13

NFDI-MatWerk Metadata Repository: Metadata Management



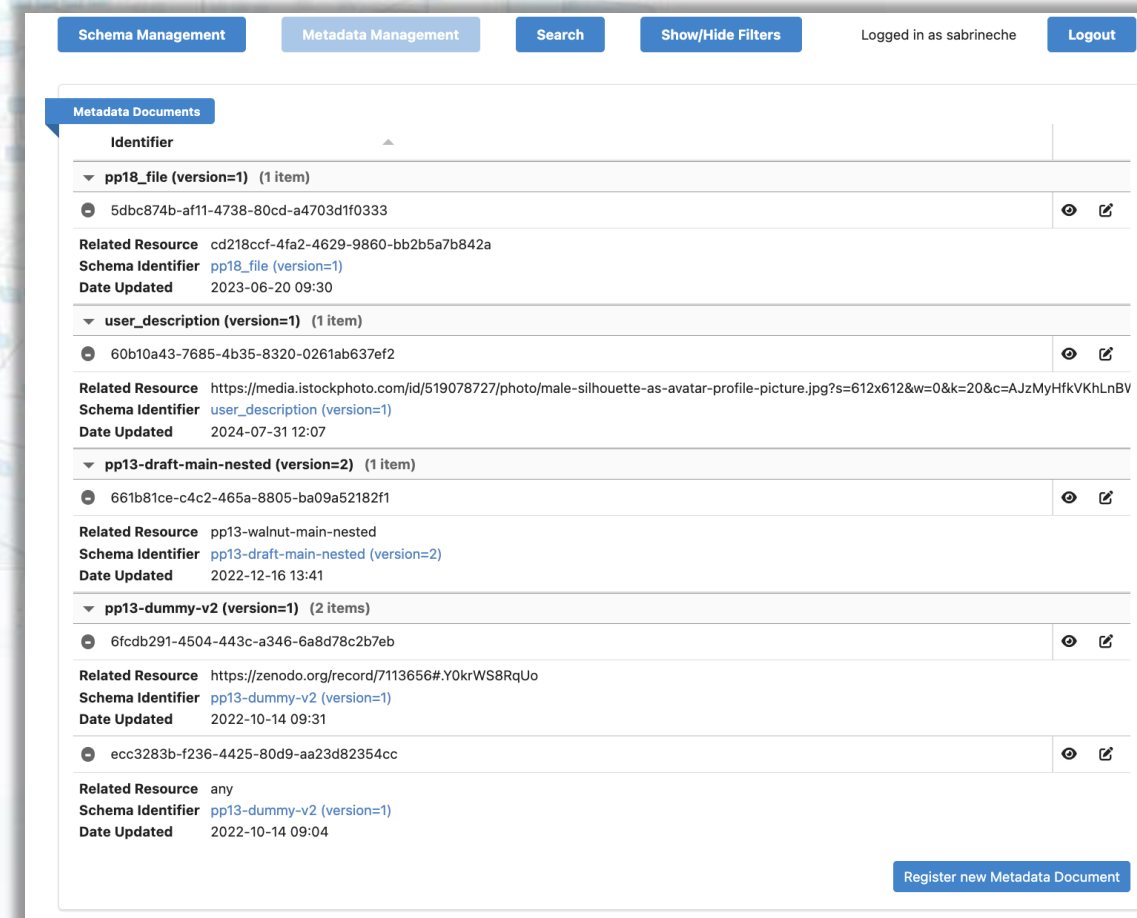
- Metadata documents are listed in a table with a column header: “identifier”.
- Filtering is also available based on “identifier”, “related resource” or “schema identifier”.
- Same functionalities, mentioned for the schema management, are also provided.
- Only metadata documents publicly available are shown if you are logged out.
- The ones created by you or shared to you are visible only after the login.

The screenshot shows the 'Metadata Management' section of the NFDI-MatWerk interface. At the top, there are navigation tabs: 'Schema Management', 'Metadata Management' (selected), 'Search', 'Show/Hide Filters', and a 'Logout' button. The user is logged in as 'sabrineche'. Below the tabs, a 'Metadata Documents' section is displayed. It contains a table with the following data:

Identifier	
▼ pp18_file (version=1) (1 item)	
5dbc874b-af11-4738-80cd-a4703d1f0333	
Related Resource cd218ccf-4fa2-4629-9860-bb2b5a7b842a	
Schema Identifier pp18_file (version=1)	
Date Updated 2023-06-20 09:30	
▼ user_description (version=1) (1 item)	
60b10a43-7685-4b35-8320-0261ab637ef2	
Related Resource https://media.istockphoto.com/id/519078727/photo/male-silhouette-as-avatar-profile-picture.jpg?s=612x612&w=0&k=20&c=AJzMyHfkVKhLnBv	
Schema Identifier user_description (version=1)	
Date Updated 2024-07-31 12:07	
▼ pp13-draft-main-nested (version=2) (1 item)	
661b81ce-c4c2-465a-8805-ba09a52182f1	
Related Resource pp13-walnut-main-nested	
Schema Identifier pp13-draft-main-nested (version=2)	
Date Updated 2022-12-16 13:41	
▼ pp13-dummy-v2 (version=1) (2 items)	
6fcd291-4504-443c-a346-6a8d78c2b7eb	
Related Resource https://zenodo.org/record/7113656#.Y0krWS8RqUo	
Schema Identifier pp13-dummy-v2 (version=1)	
Date Updated 2022-10-14 09:31	
ecc3283b-f236-4425-80d9-aa23d82354cc	
Related Resource any	
Schema Identifier pp13-dummy-v2 (version=1)	
Date Updated 2022-10-14 09:04	

At the bottom right of the interface, there is a button labeled 'Register new Metadata Document'.

- Task: Change ACL permission, add License and search for your uploaded metadata document.



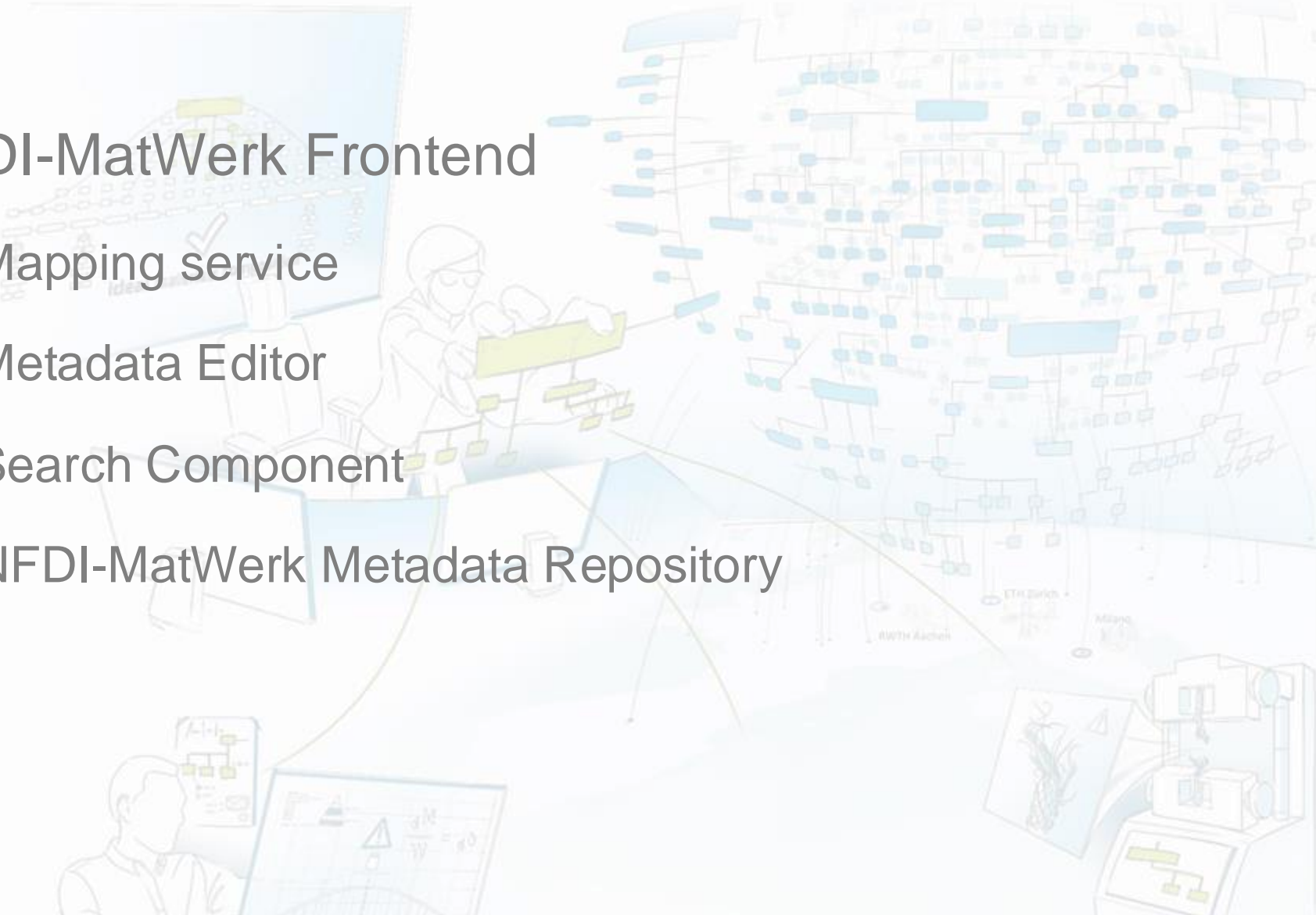
The screenshot displays the NFDI MatWerk Metadata Management interface. The top navigation bar includes tabs for Schema Management, Metadata Management, Search, and Show/Hide Filters. The user is logged in as 'sabrineche' and can click 'Logout'. The main content area is titled 'Metadata Documents' and lists several documents with their identifiers, related resources, schema identifiers, and update dates. Each document entry includes a trash icon and an edit icon.

Identifier	Related Resource	Schema Identifier	Date Updated
pp18_file (version=1) (1 item)			
5dbc874b-af11-4738-80cd-a4703d1f0333	cd218ccf-4fa2-4629-9860-bb2b5a7b842a	pp18_file (version=1)	2023-06-20 09:30
user_description (version=1) (1 item)			
60b10a43-7685-4b35-8320-0261ab637ef2	https://media.istockphoto.com/id/519078727/photo/male-silhouette-as-avatar-profile-picture.jpg?s=612x612&w=0&k=20&c=AJzMyHfkVKhLnBv	user_description (version=1)	2024-07-31 12:07
pp13-draft-main-nested (version=2) (1 item)			
661b81ce-c4c2-465a-8805-ba09a52182f1	pp13-walnut-main-nested	pp13-draft-main-nested (version=2)	2022-12-16 13:41
pp13-dummy-v2 (version=1) (2 items)			
6fcd291-4504-443c-a346-6a8d78c2b7eb	https://zenodo.org/record/7113656#.Y0krWS8RqUo	pp13-dummy-v2 (version=1)	2022-10-14 09:31
ecc3283b-f236-4425-80d9-aa23d82354cc	any	pp13-dummy-v2 (version=1)	2022-10-14 09:04

Register new Metadata Document

Conclusions

- NFDI-MatWerk Frontend
 - Mapping service
 - Metadata Editor
 - Search Component
- NFDI-MatWerk Metadata Repository



Acknowledgements

Contributions:

Thomas Jejkal, Andrea Recchia

Used material:

<https://github.com/kit-data-manager/mapping-service>

<https://metadata-editor.gitlab.io/documentation/>

<https://kit-data-manager.github.io/webpage/metastore/index.html>

Founded by:

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