



Experimental data transfer system BENTEN at SPRING-8

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Japan Synchrotron Radiation Research Institute (JASRI)

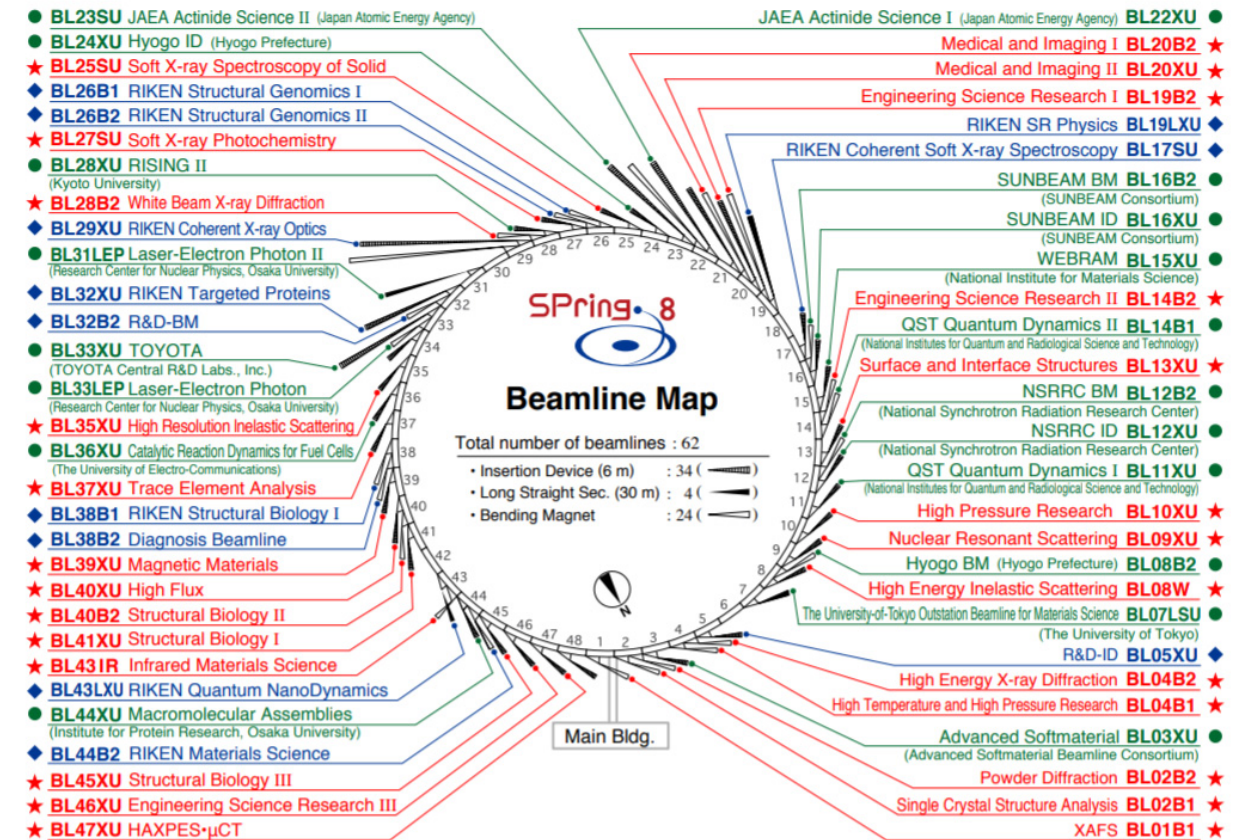
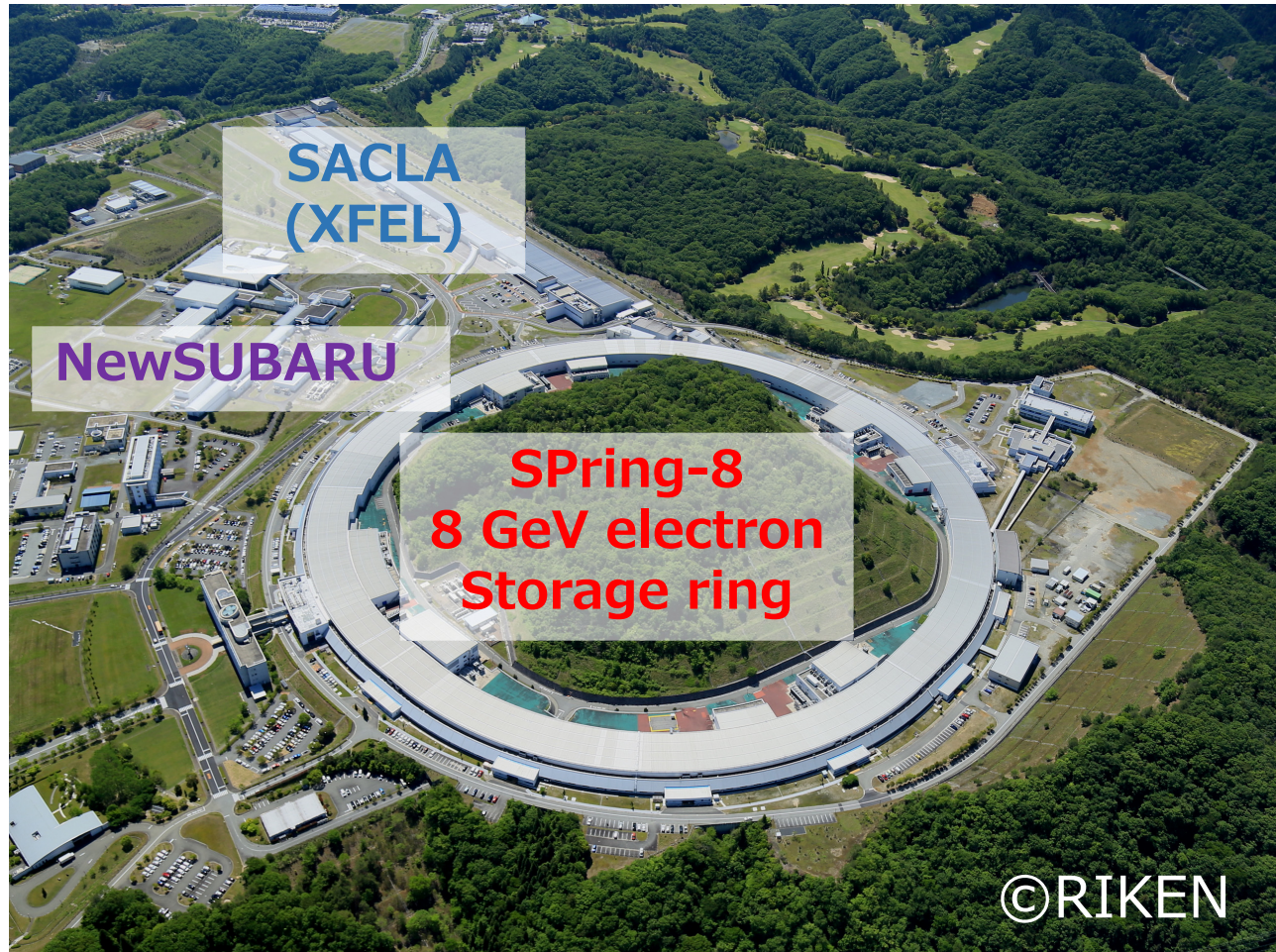
8th October, 2019



- Introduction
- Experimental data transfer system BENTEN
- Operation of BENTEN at SPring-8
- Summary and Future plan

Introduction

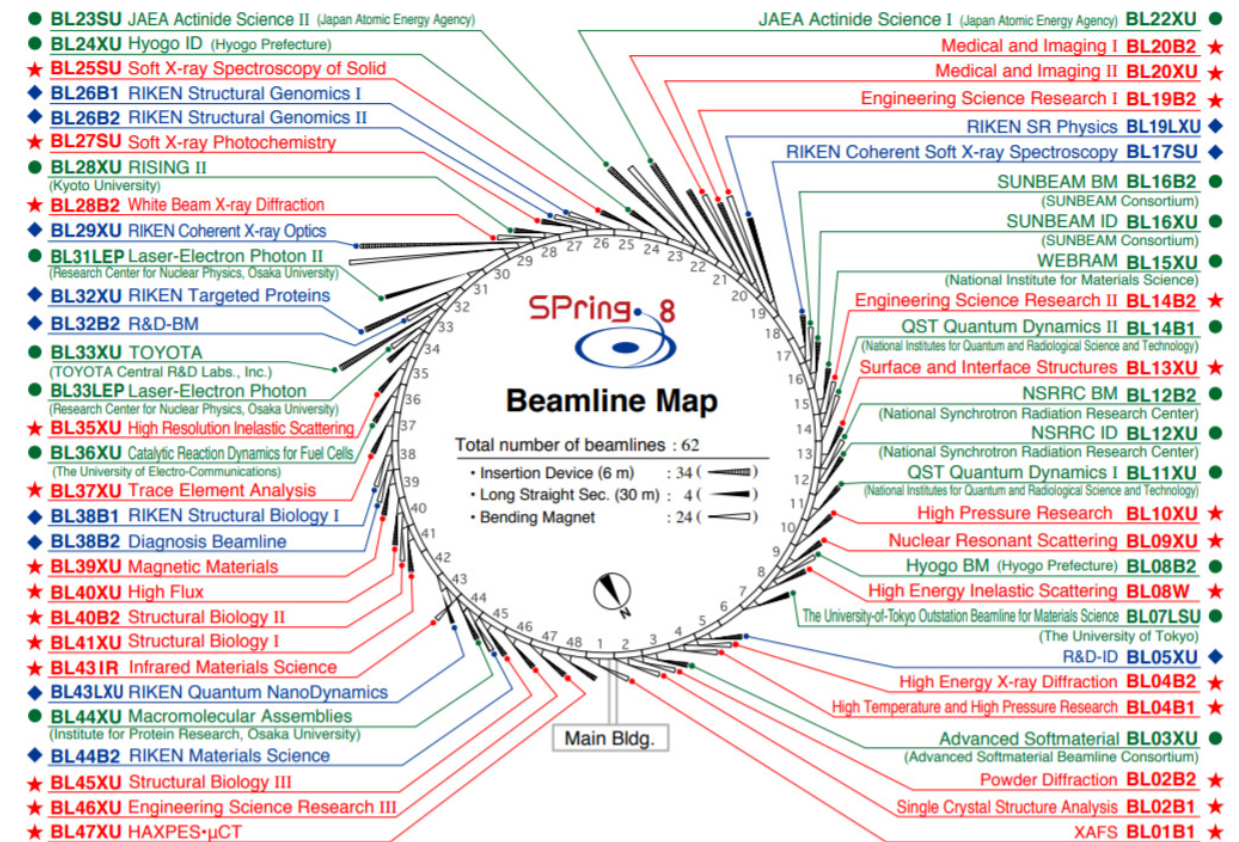
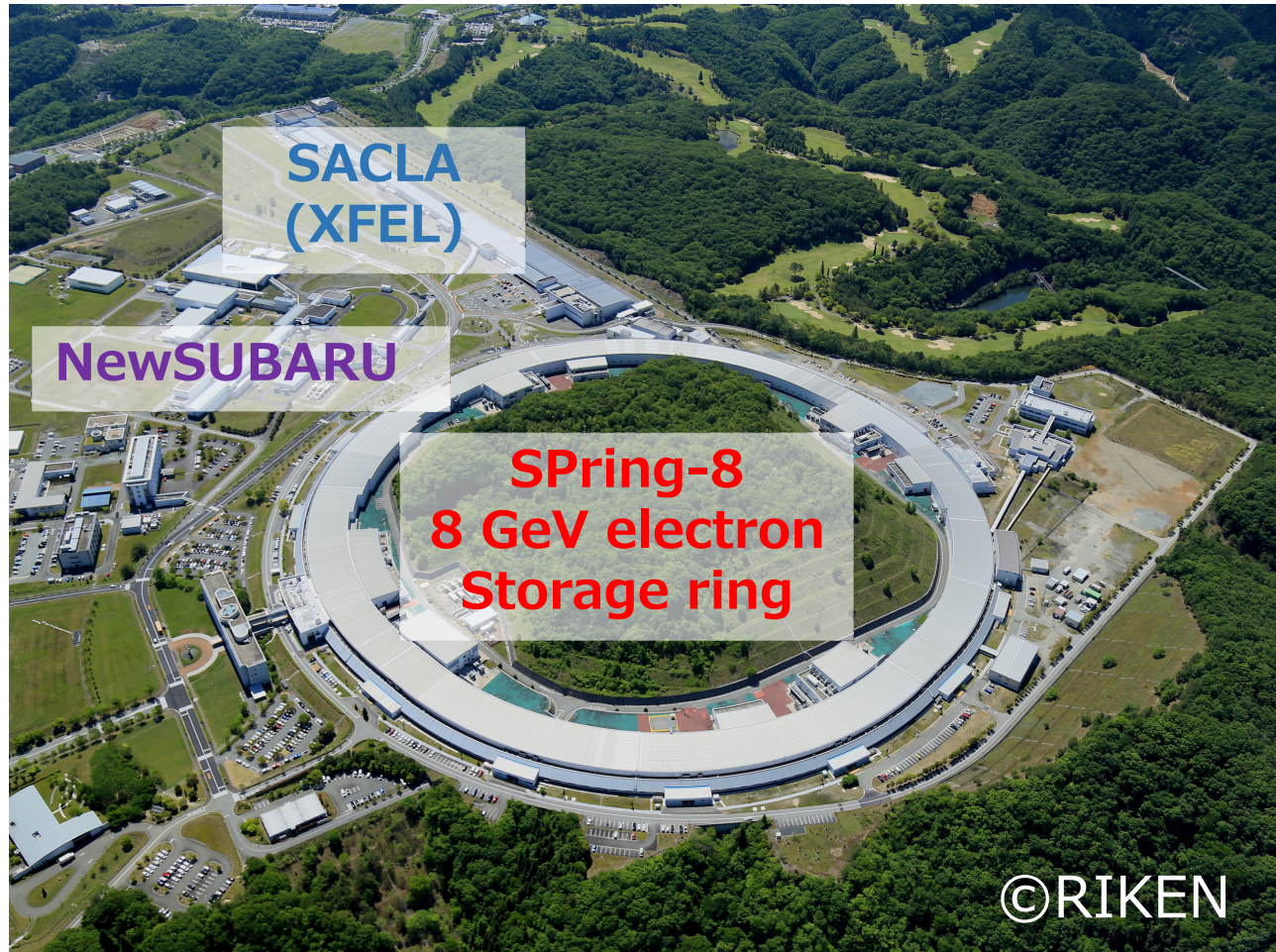
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- In total, ~17,000 users/year come to SPring-8 for experiments



Experimental stations in 57 beamlines

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- ➔ Required Experimental data transfer for Data access through the Internet



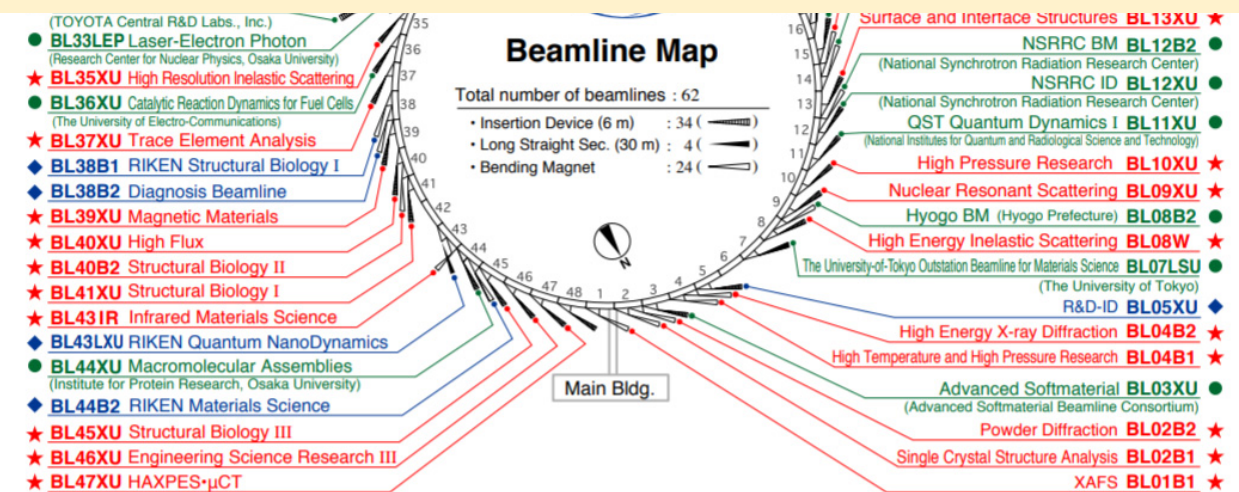
Experimental stations in 57 beamlines

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- Data science such as material informatics
- ➔ Recently attracting public attentions



Experimental stations in 57 beamlines

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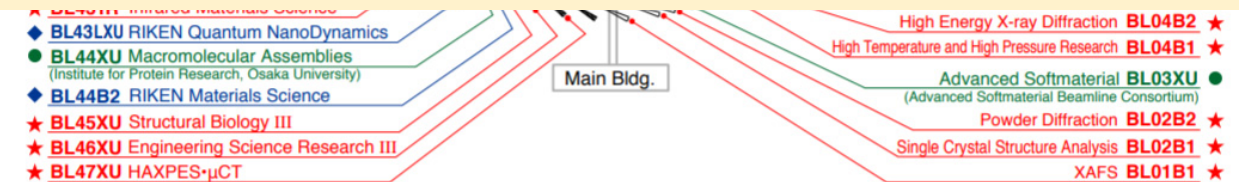
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- **Restricted data access**

- Remote experiment
- Proxy measurements

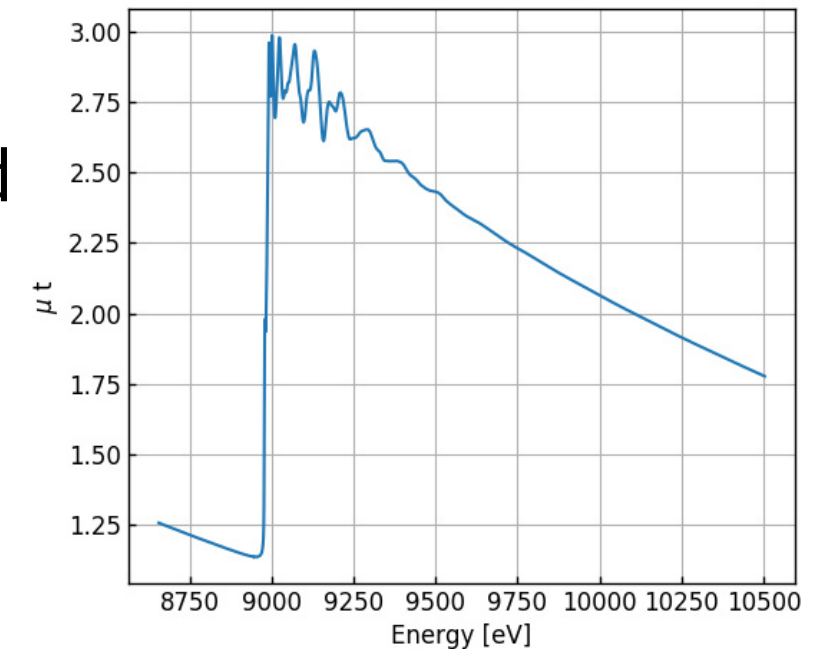


Experimental stations in 57 beamlines

An example of open data at SPring-8

- XAFS spectrum data for Standard sample
 - **XAFS**: X-ray Absorption Fine Structure
 - ~ 800 measured data at SPring-8: 2nd in the world
 - Utilized as reference for the measurement

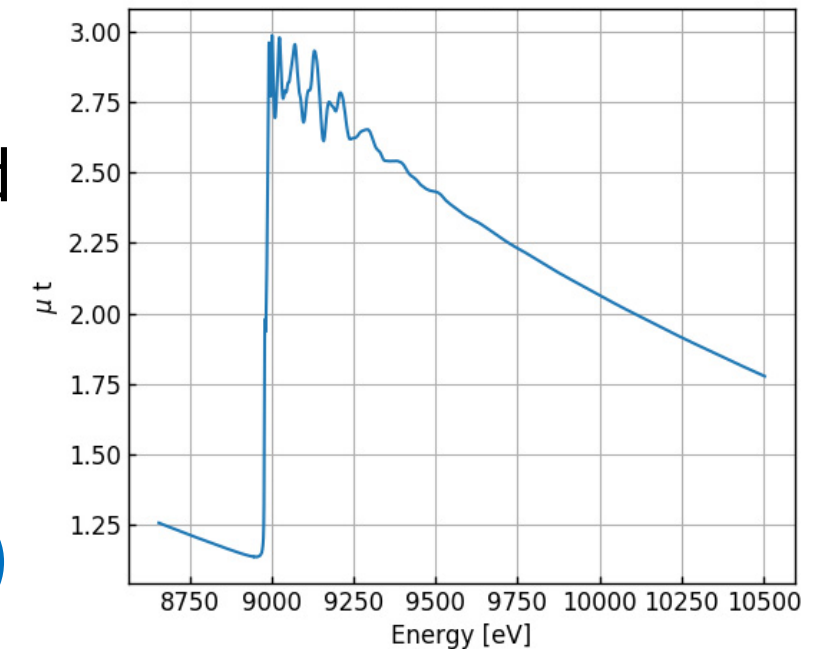
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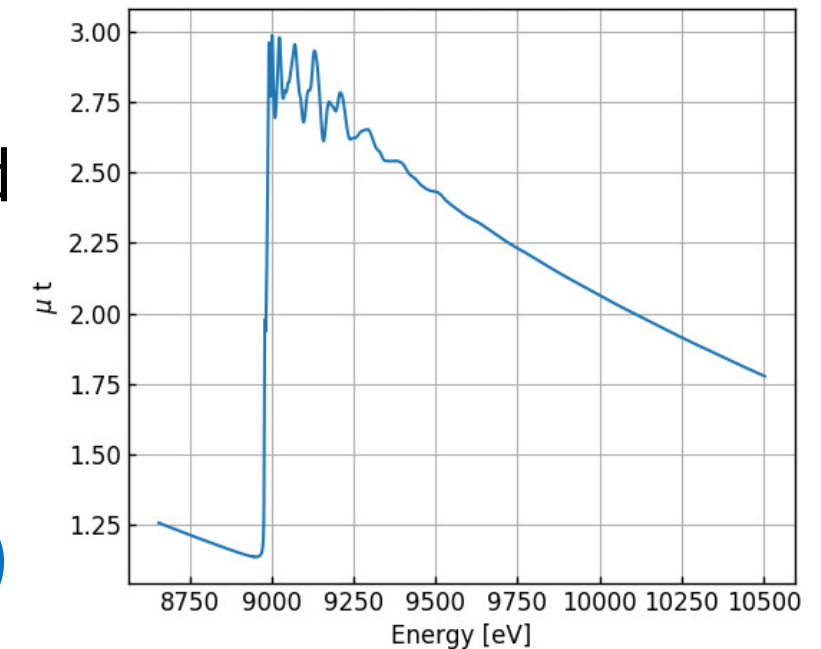
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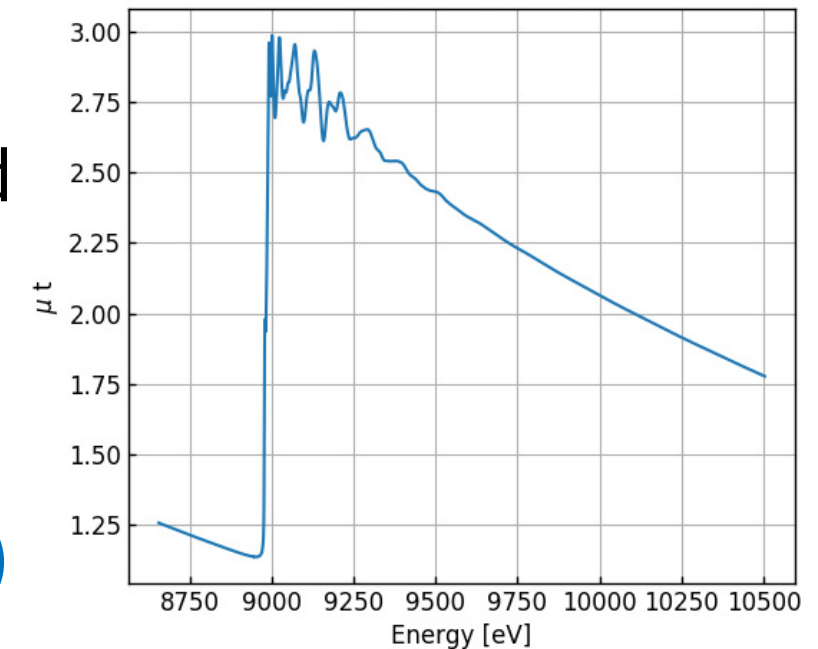
Experimental data transfer system BENTEN

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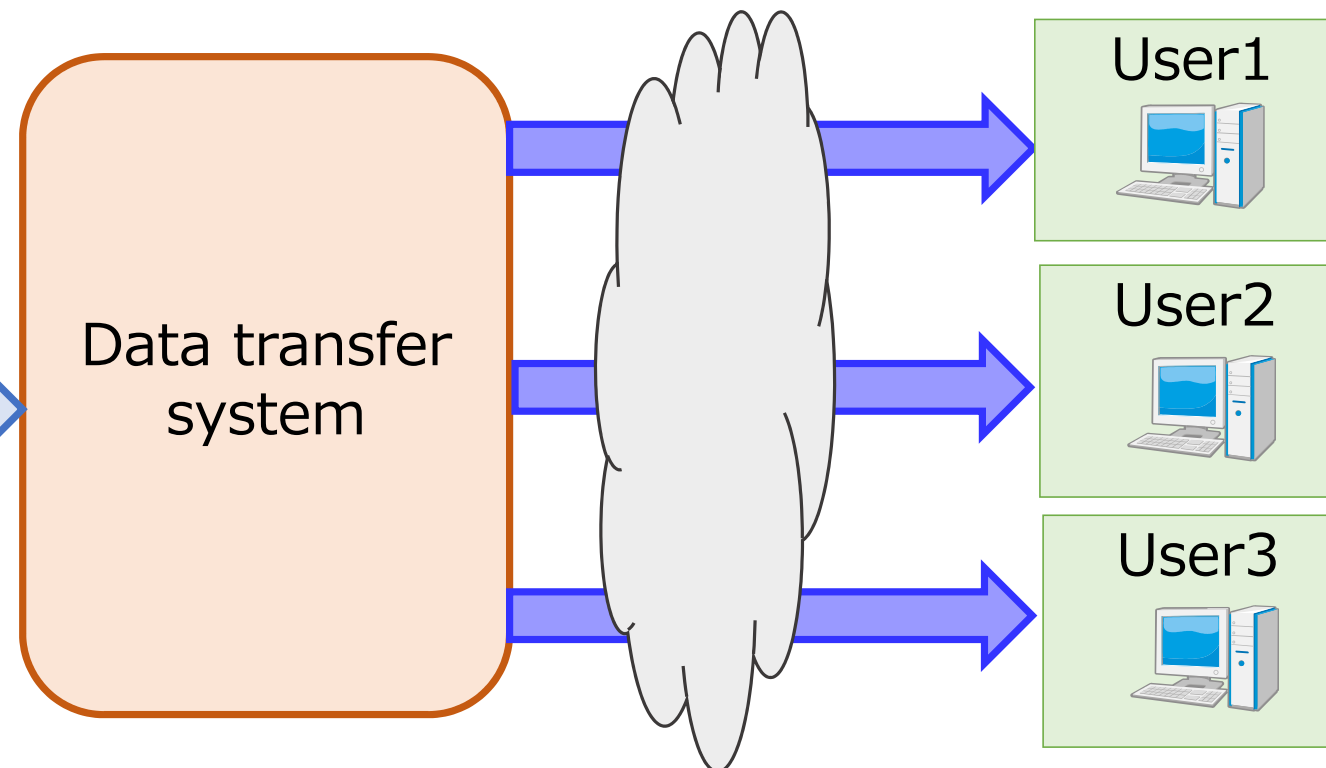
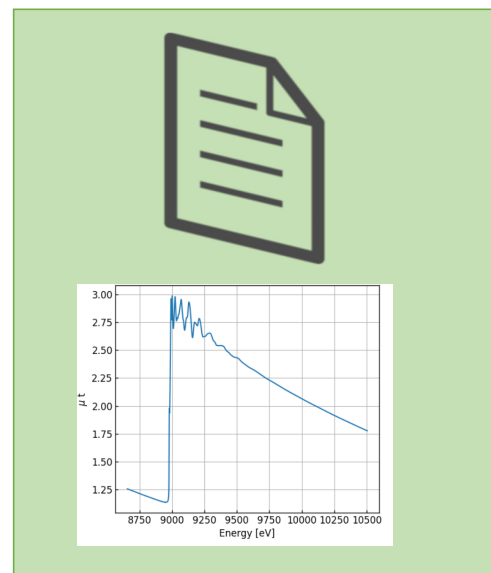
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- Control range of data sharing
 - **Case1: Open data access**

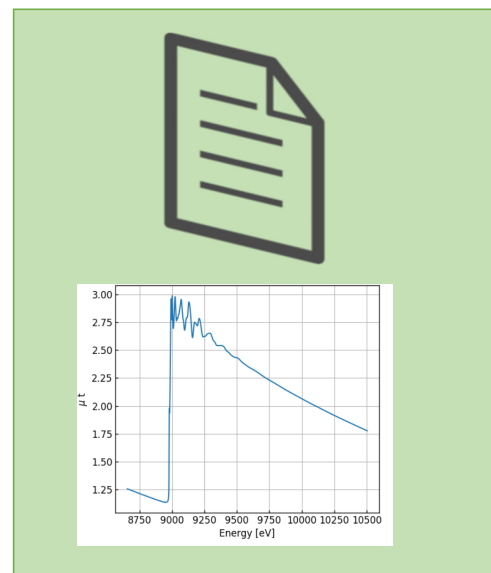
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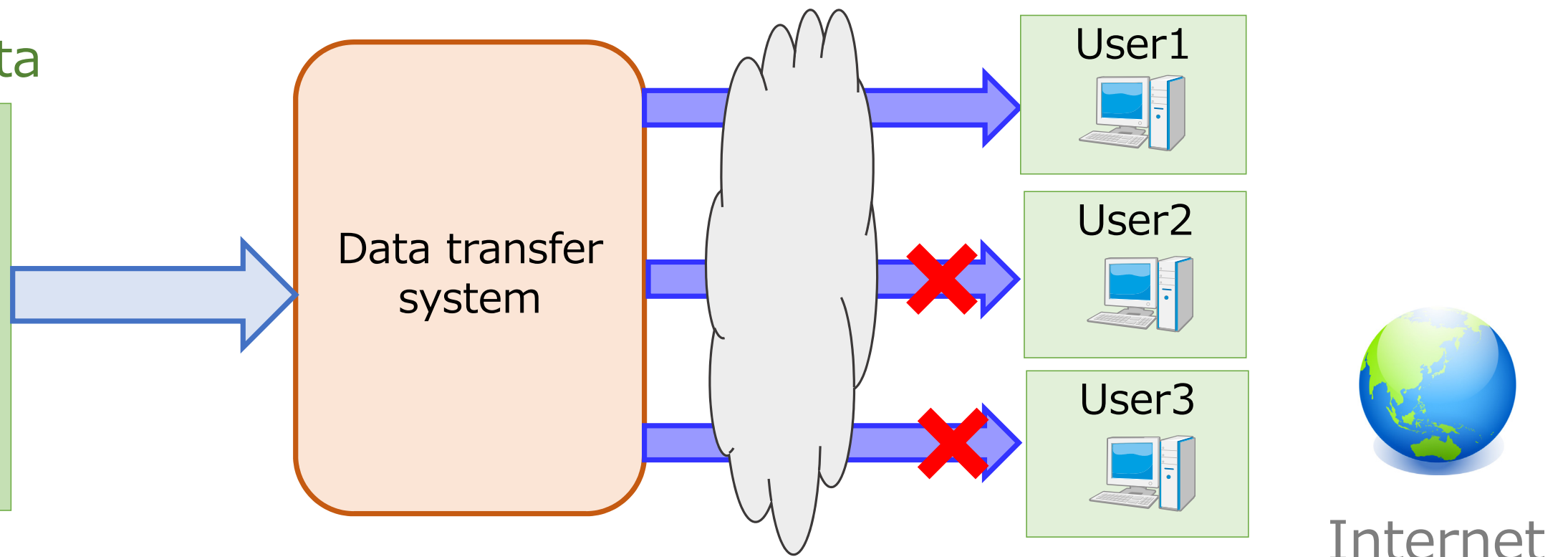
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 - **Case2: Restricted data access**

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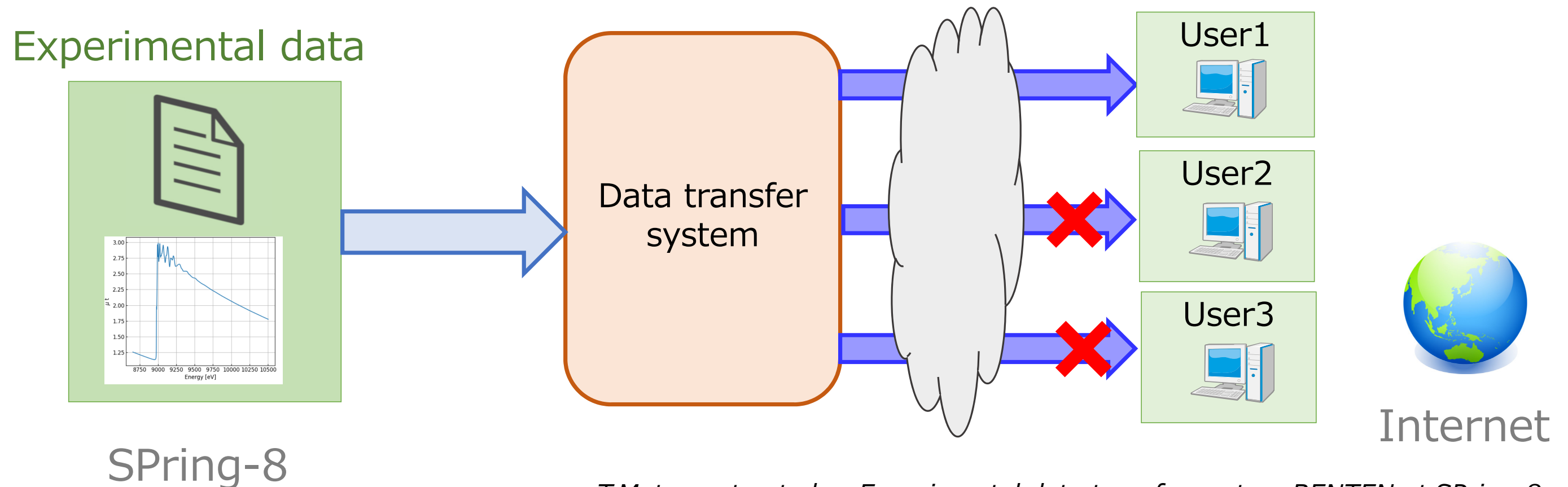


SPring-8



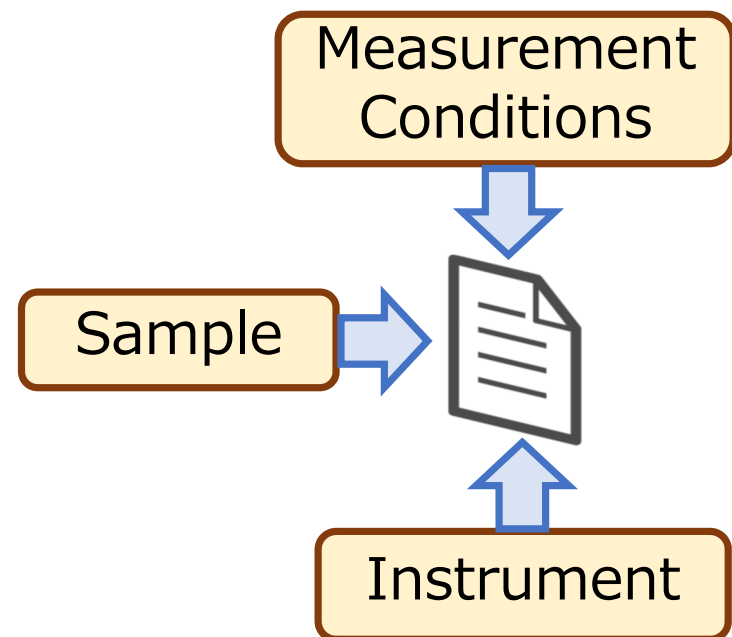
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- Control range of data sharing → **Authentication**
 - **Case2: Restricted data access**



Requirements in Experimental data transfer (2)

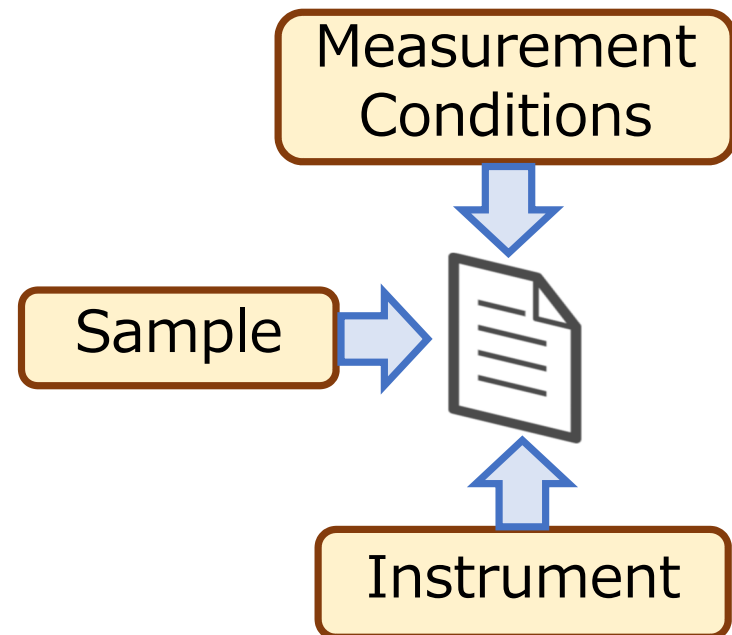
- Metadata management



- Easy to describe metadata in the experiments
 - To provide sufficient metadata to utilize data
 - Automated metadata extraction is desired

Requirements in Experimental data transfer (2)

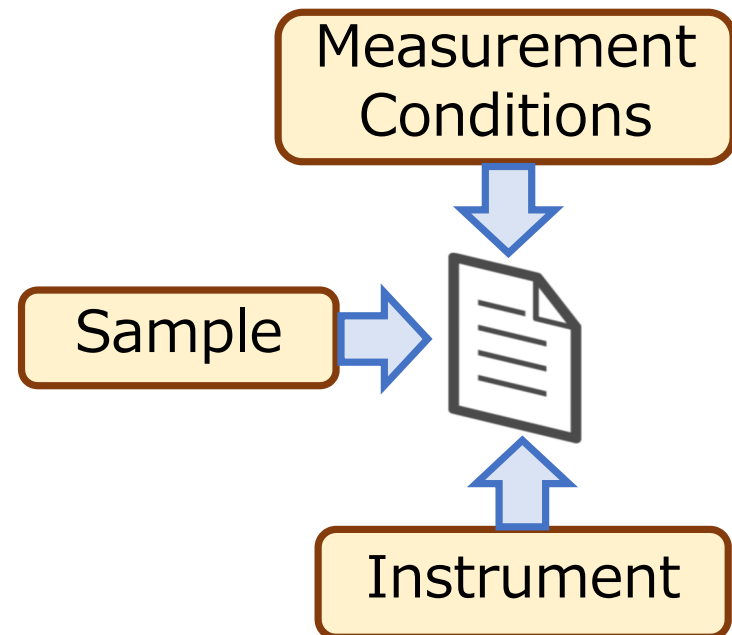
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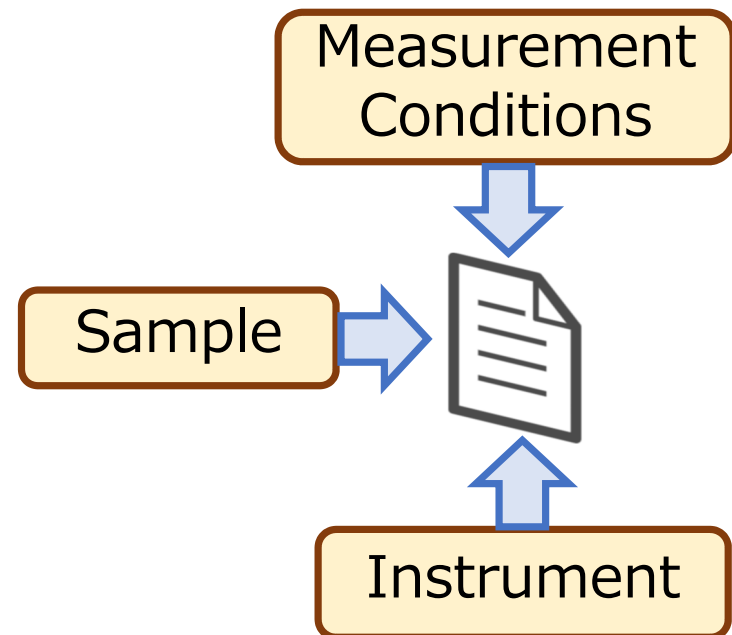
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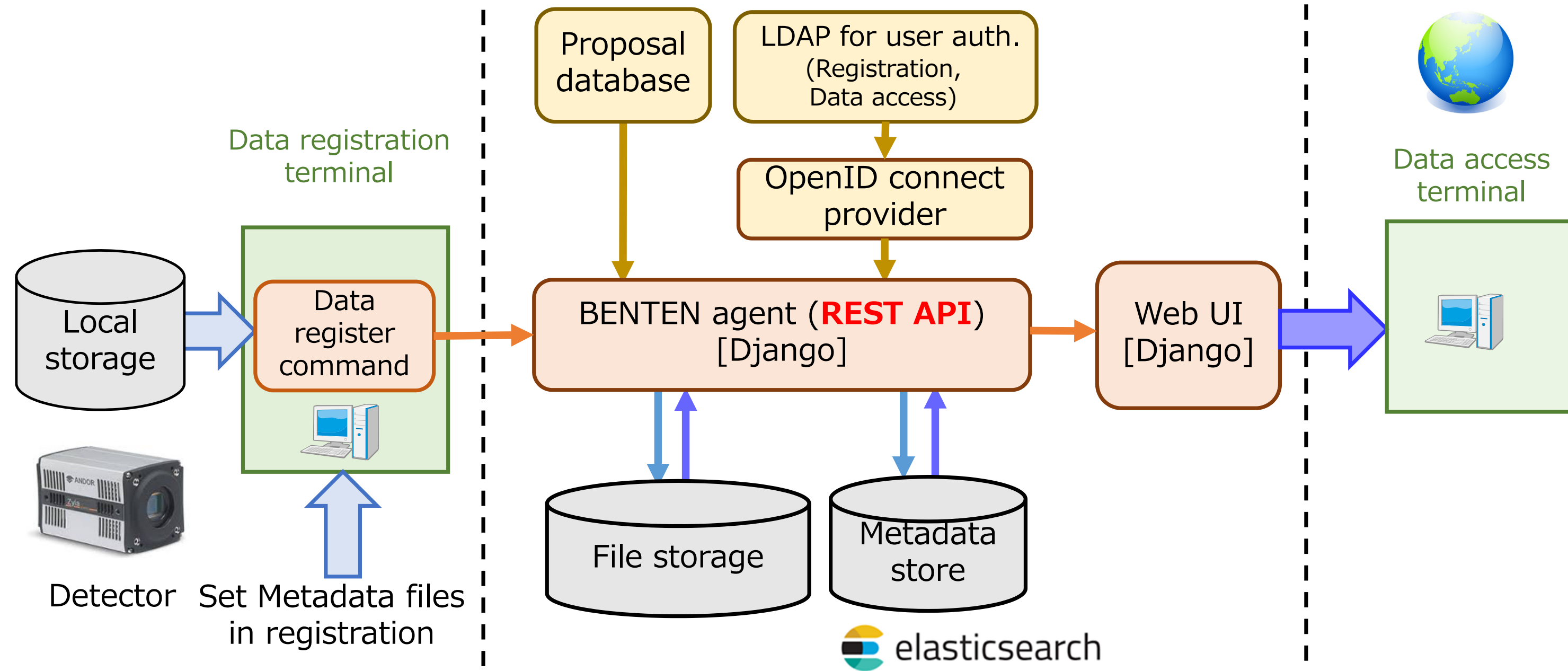
- Data life cycle
 - Create, Update, Open/Closed access, Delete
- Define items for Open Data
 - PID (Persistent ID), Contact name and its affiliation

BENTEN system Overview

Experimental station

BENTEN system

User

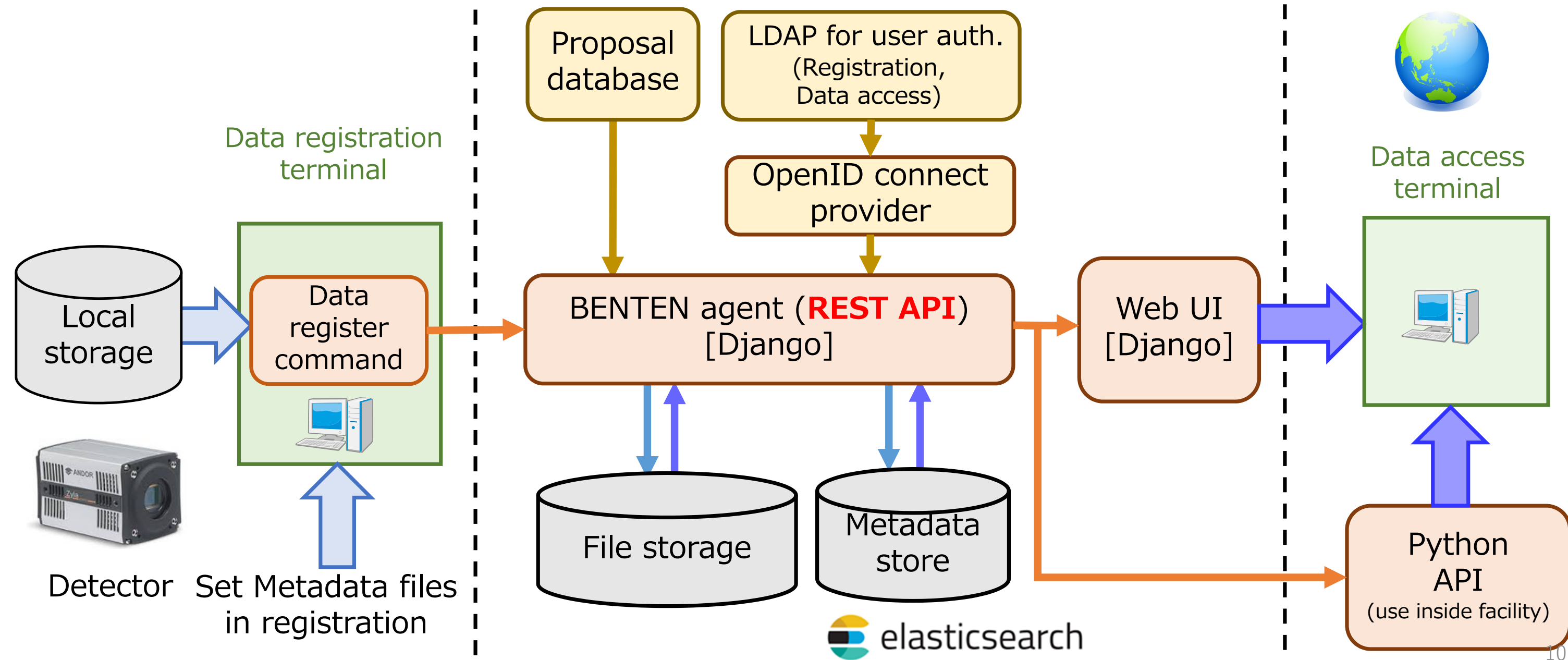


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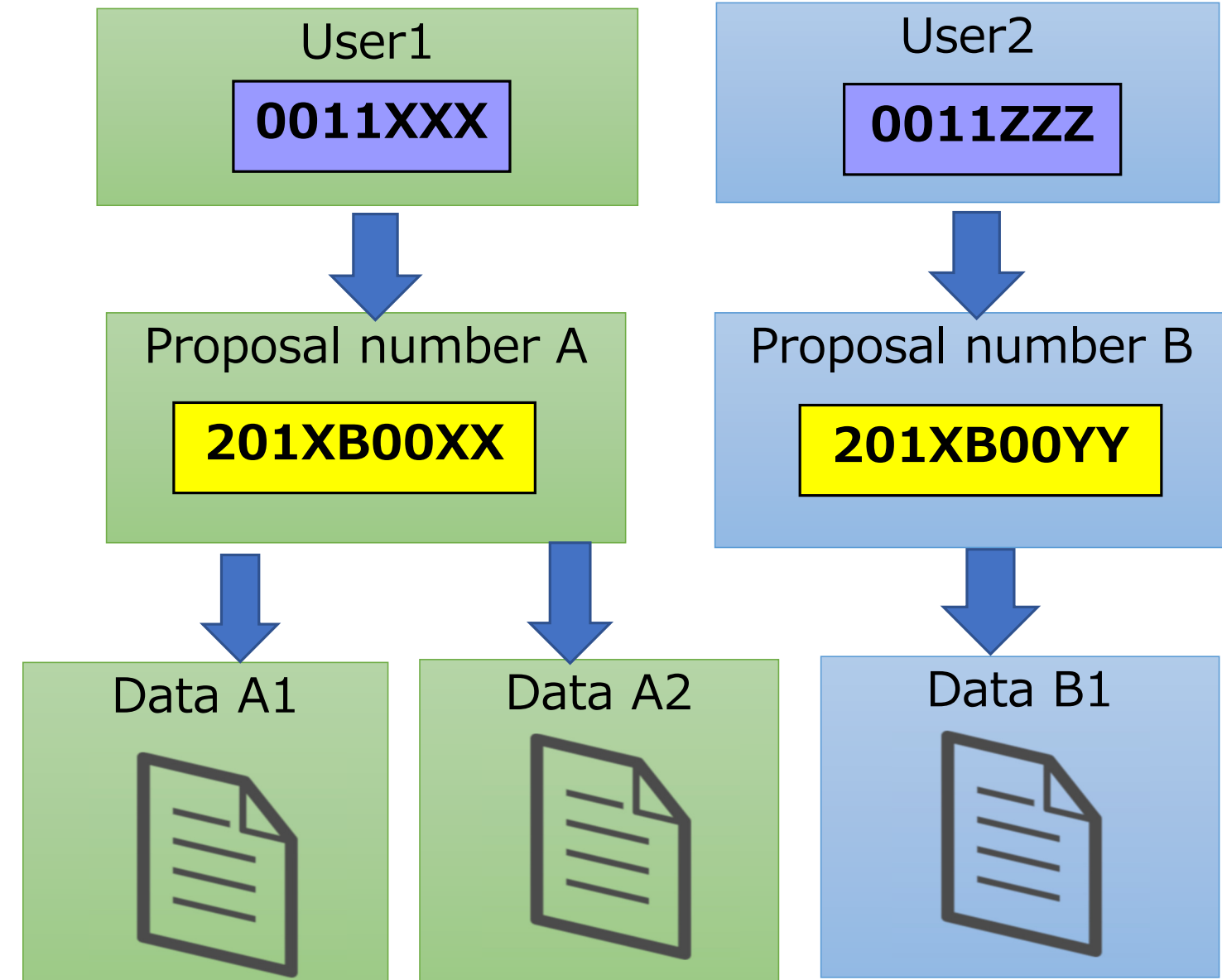
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Authorization for data access

OpenID connect 1.0
for authentication

How to control
range for data sharing?

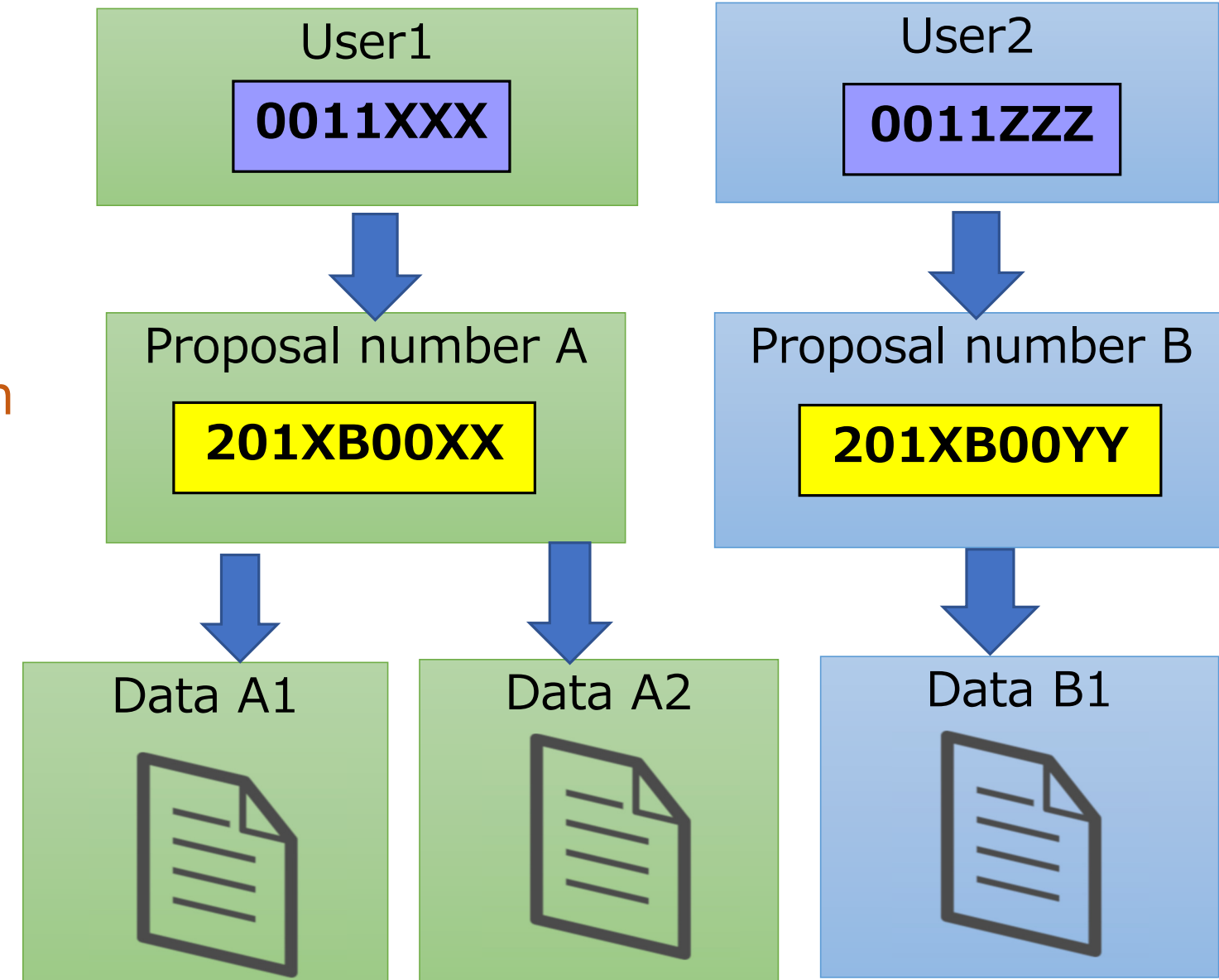


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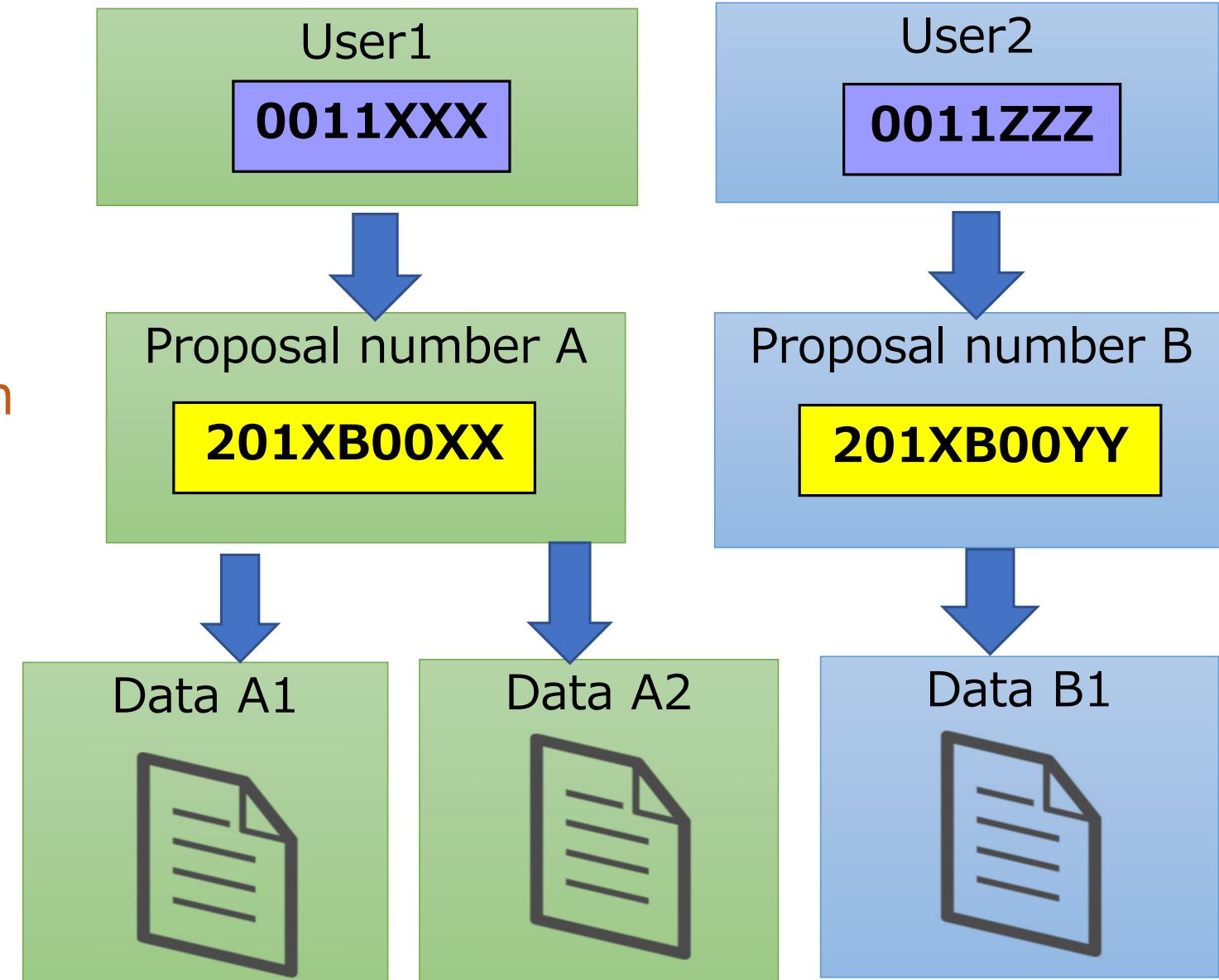


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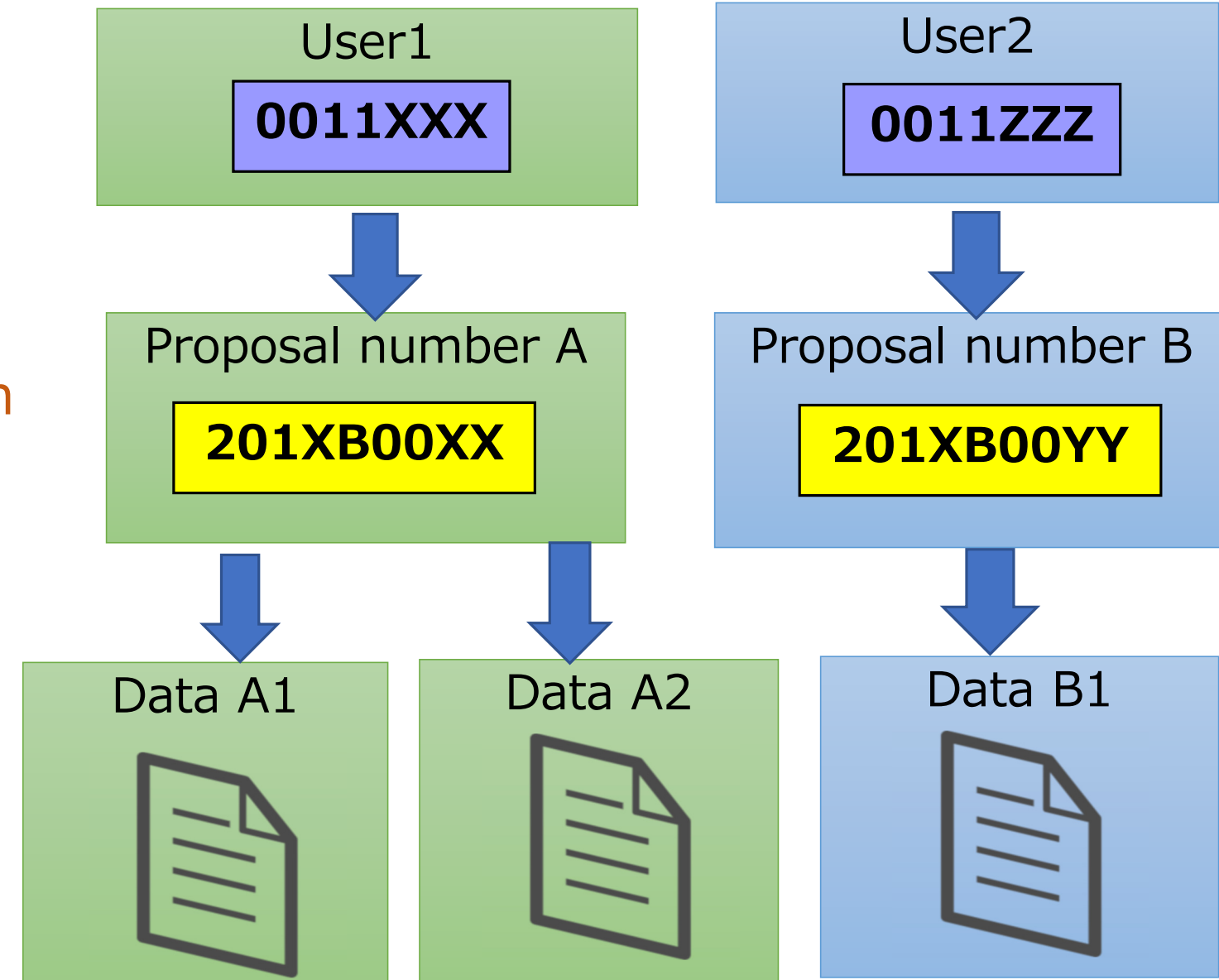


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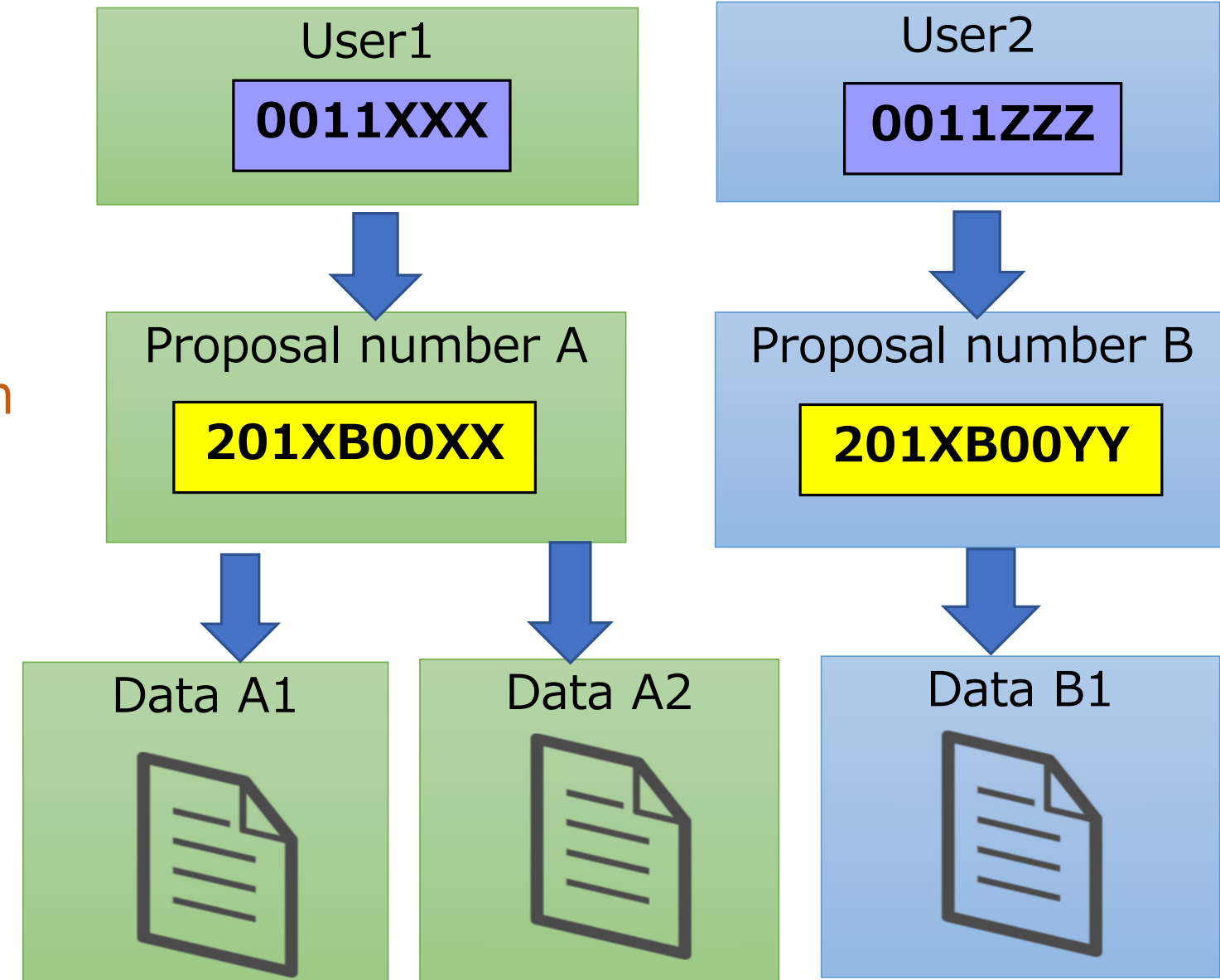


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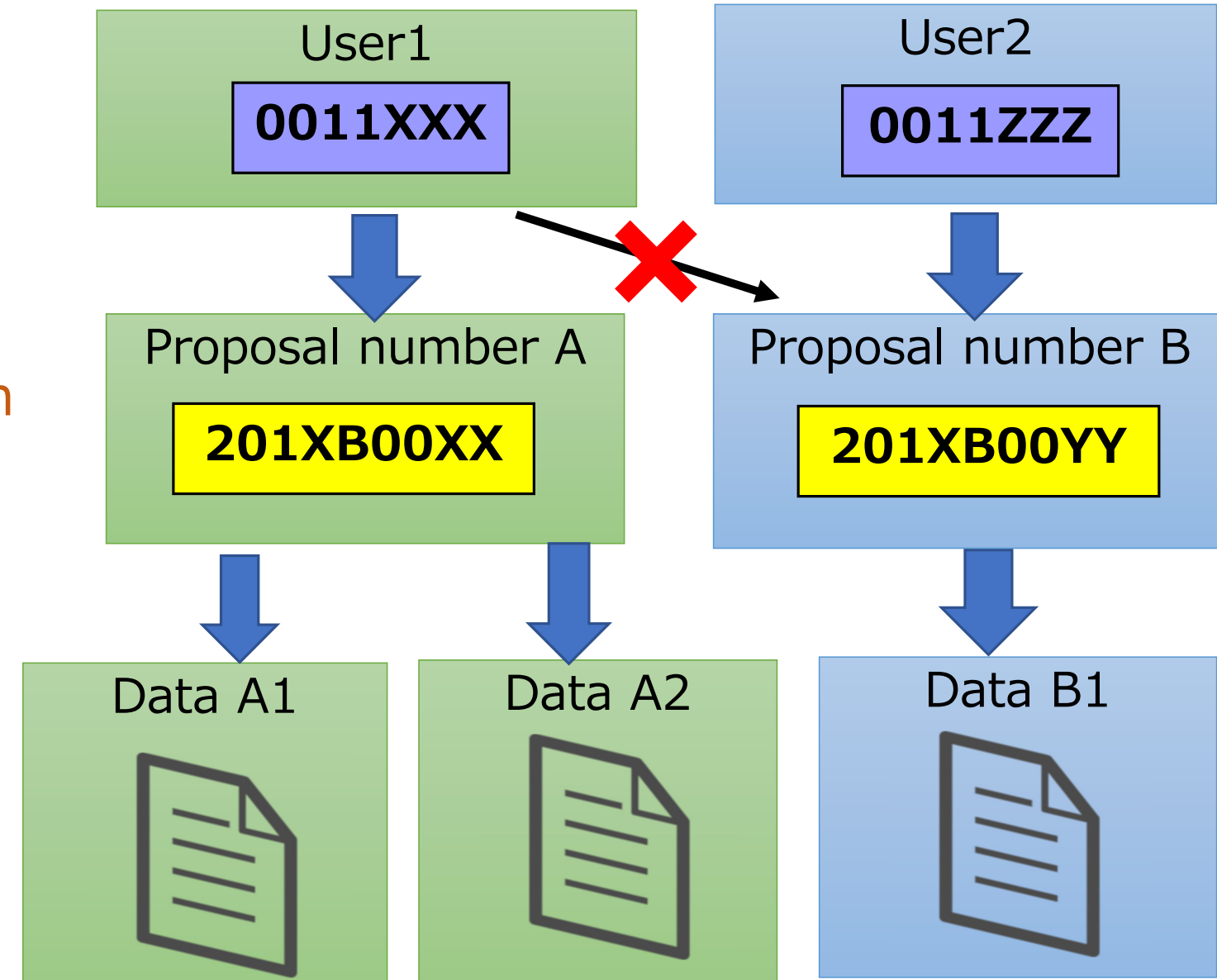


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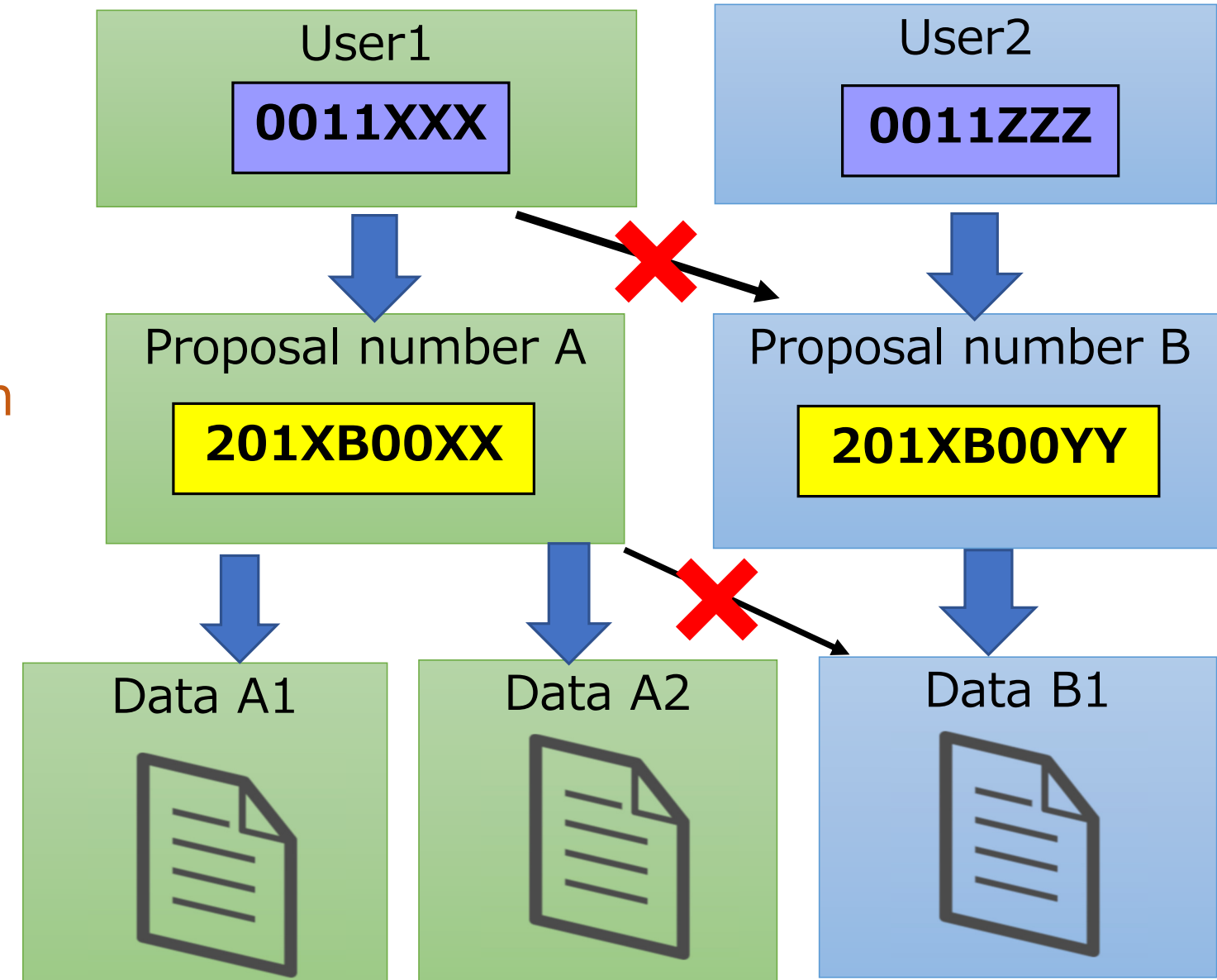


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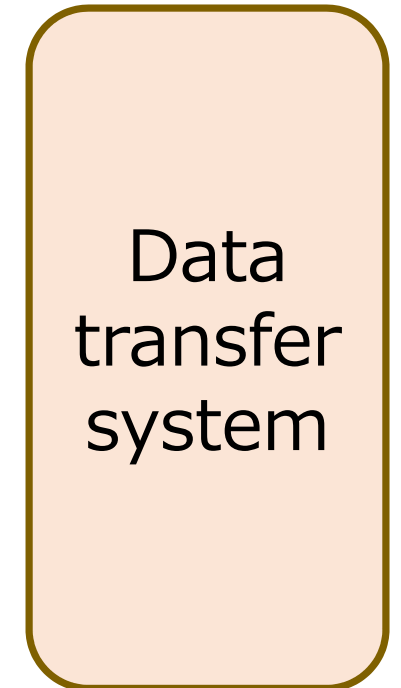
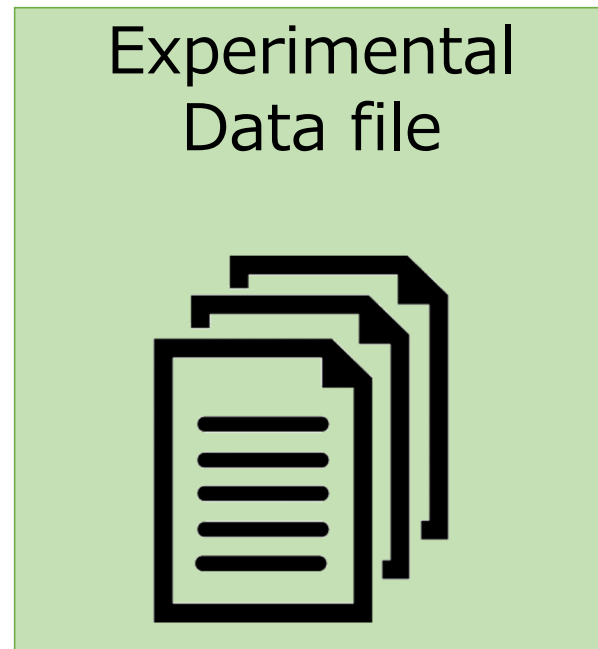
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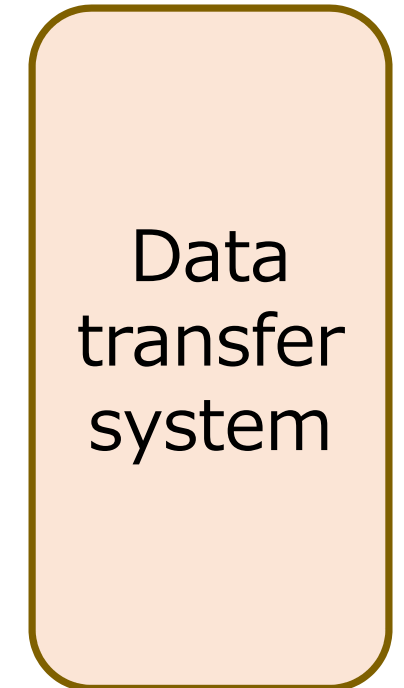
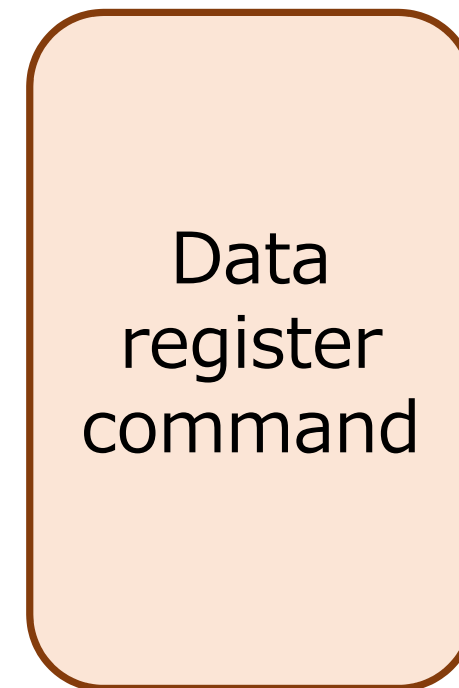
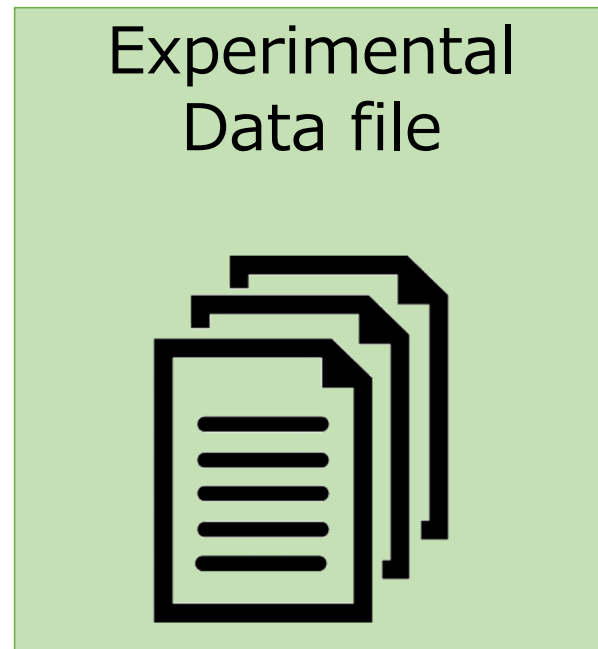
Our approach to Metadata

- To describe metadata, common data format is desired
 - ex.) Nexus format based on HDF5 data container



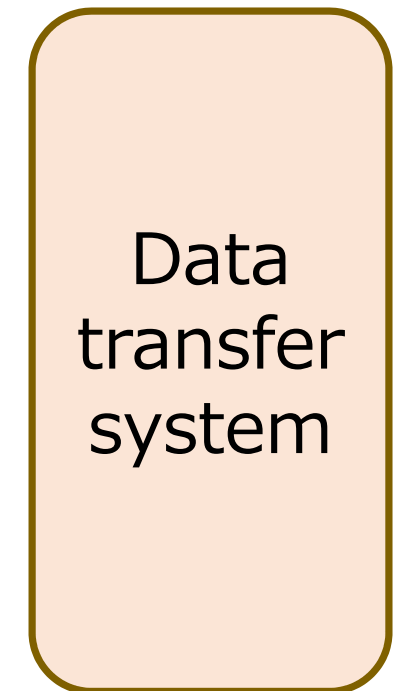
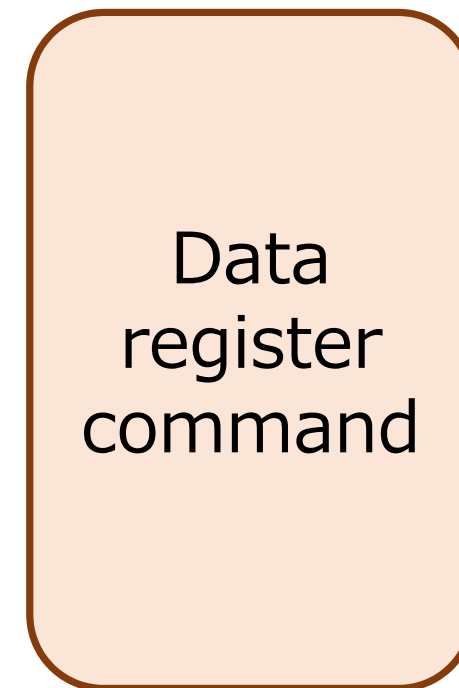
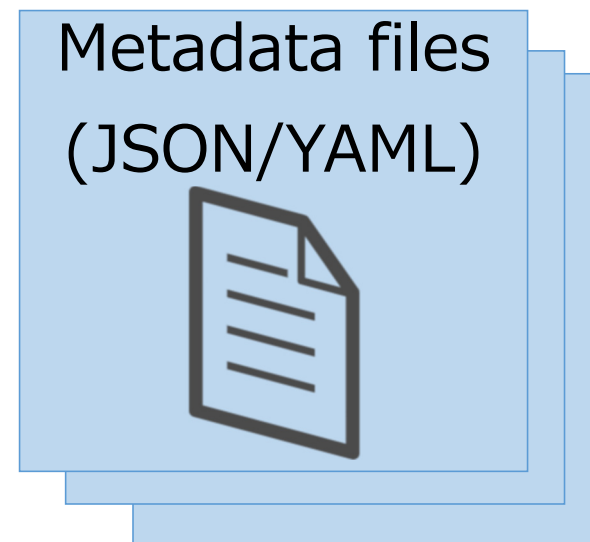
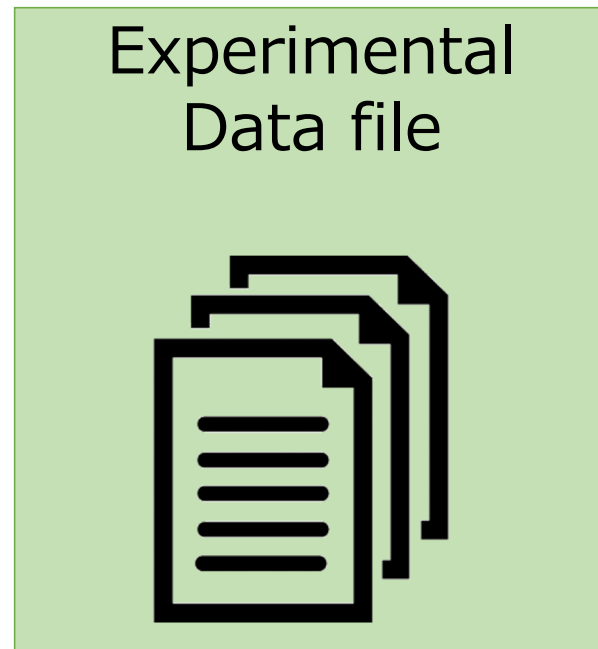
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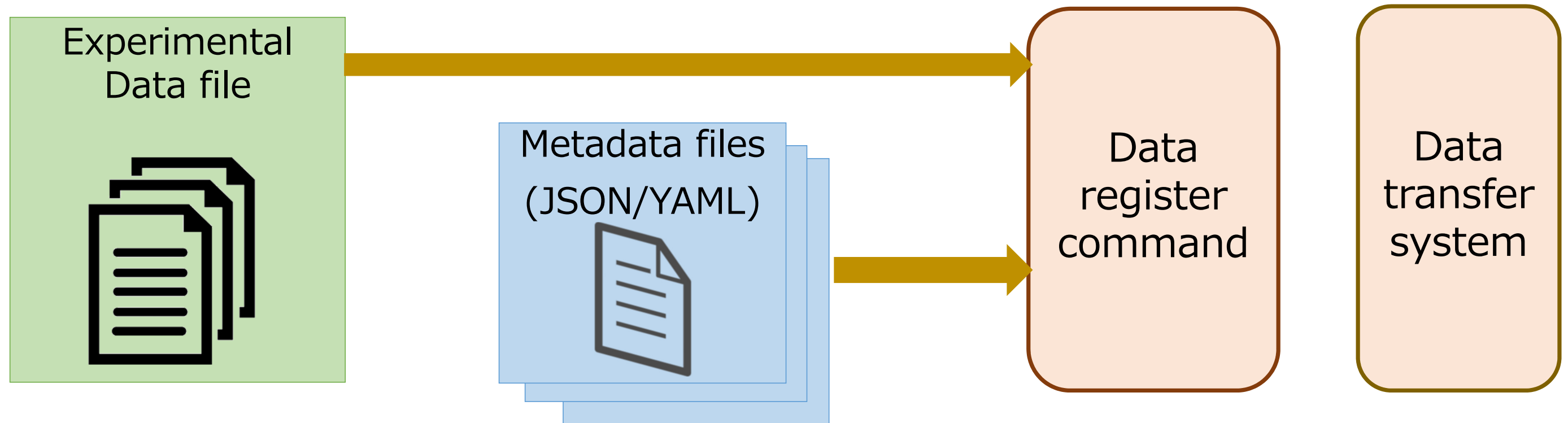
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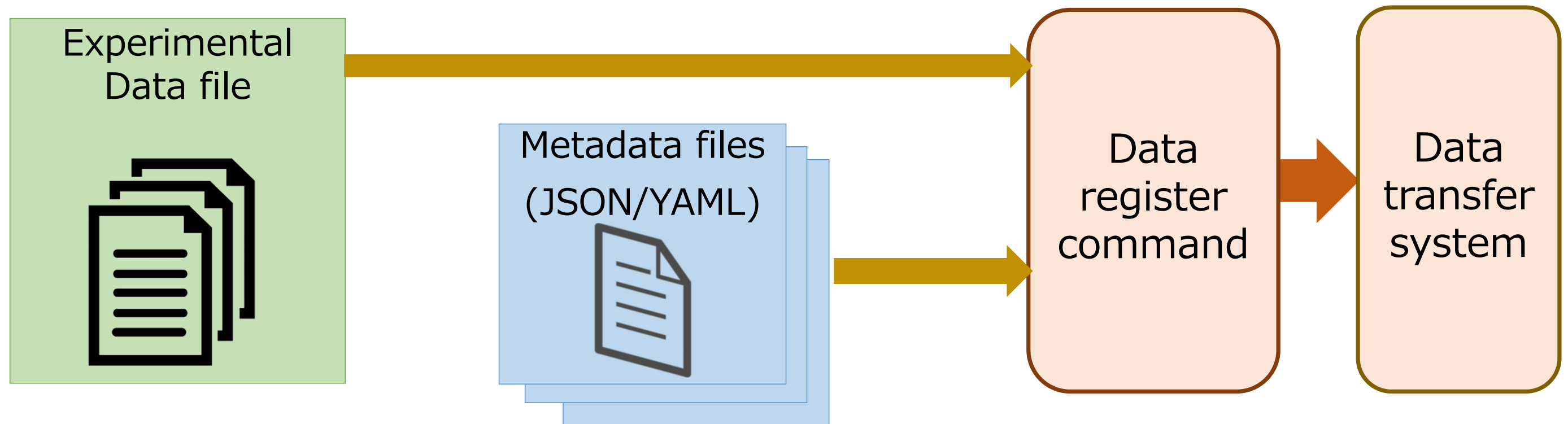
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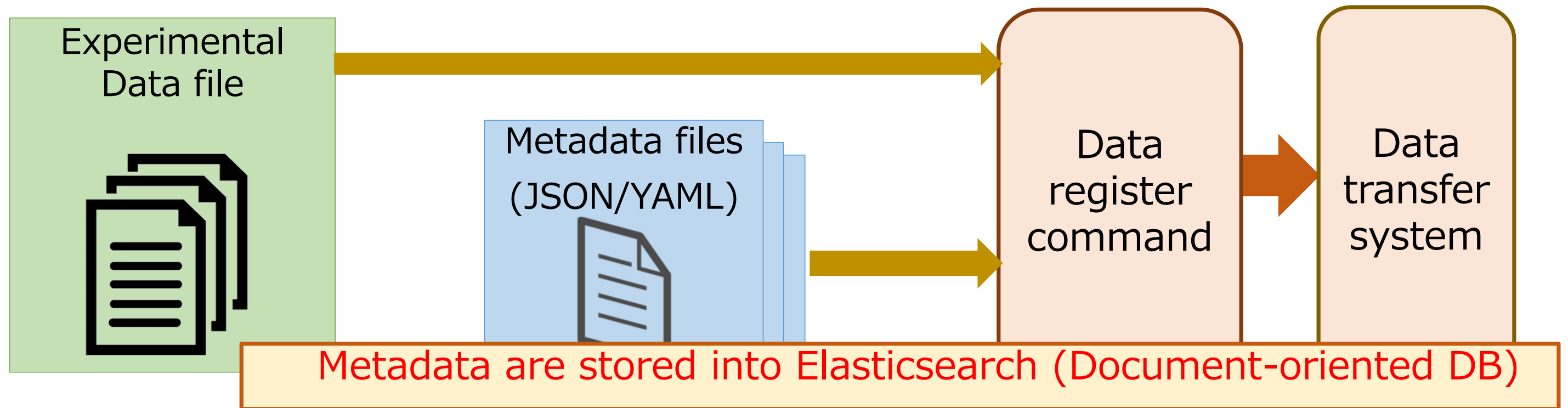
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Metadata description by User

```
sample:
  name: Cupper (1) oxide
  chemical_formula: Cu2O
  element:
    - name: Cu
      suffix: 2
    - name: O
      suffix: 1
  vendor: KOJUNDO CHEMICAL LABORATORY
  model_number: CU01PB
measurement:
  method:
    name: XAFS
    detection: Transmission
    absorption_edge: Cu K-edge
  date:
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- User prepares metadata in files with JSON or YAML
 - Human/Machine readable

Ex.) Metadata with YAML

Metadata description by User

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  element:  
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      suffix: 2  
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Sample category

Possible to define array

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 - Possible to define hierarchical structure
- User can add items required for measurements

Ex.) Metadata with YAML

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- First attempt:
 - Restricted data access for user experiments at BL14B2
 - Automated data transfer with BENTEN was implemented
 - Open data access for XAFS standard sample
 - Registered offline with sufficient metadata
 - Major items were automatically extracted
 - However, manual input was still required (sample, instrument etc.)

Web portal (Accessible data for user)

SPring-8 Experimental Data Transfer System UID: 0000664 LOGOUT

Zr Search under folder your proposal DOWNLOAD CHECKED ITEMS

root
 SPring-8
 BL14B2
 Standard
 Zr
 K
 311
 stabilized_ZrO2_YSZ_ (selected)
 stabilized_ZrO2_MSZ_
 stabilized_ZrO2_CSZ_
 approx_ZrSiO4
 Zr_SO4_2_4H2O
 Zr_OH_4
 ZrSi2
 ZrS2
 ZrO_NO3_2_2H2O
 ZrO_CH3COO_2
 ZrOCl2_8H2O
 ZrO2
 ZrN
 ZrI4

| FILE NAME | PATH |
|--|--|
| <input checked="" type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ_Si311_50ms_170419_fe.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ_Si311_50ms_170419_fe.system.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ_Si311_50ms_170419_fe.user.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> README.csv | //SPring-8/BL14B2/Standard K_stabilized_ZrO2_ |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ_Si311_50ms_170419.dat | //SPring-8/BL14B2/Standard |

| | |
|-------------------------------------|--|
| @subject@correspondance@affiliation | JASRI |
| @subject@create_time | 2019-03-27 21:23:47 |
| @subject@disk_name | Standard |
| @subject@facility | SPring-8 |
| @subject@pid | spring8.32caaefe-e665-494b-e |
| @subject@proposal_number | 2014S0000 |
| @subject@register_name | /SPring-8/BL14B2/Standard/Zr/K/311/s K_stabilized_ZrO2_YSZ_Si3' |
| @subject@representative@username | 0007719 |

Web portal (Accessible data for user)

The screenshot displays the SPring-8 Experimental Data Transfer System interface. At the top, the logo and name 'SPring-8 Experimental Data Transfer System' are visible on the left, and the user ID 'UID: 0000664' and a 'LOGOUT' button are on the right. Below the header, there is a search bar containing 'Zr', a 'Search under folder' button, a dropdown menu showing 'your proposal', and a 'DOWNLOAD CHECKED ITEMS' button.

The main content area is divided into two panels. The left panel shows a directory tree in an 'explore' style. The path is: root > SPring-8 > BL14B2 > Standard > Zr > K > 311. The folder 'stabilized_ZrO2_YSZ_' is selected and highlighted in blue. Other folders listed include 'stabilized_ZrO2_MSZ_', 'stabilized_ZrO2_CSZ_', 'approx_ZrSiO4', 'Zr_SO4_2_4H2O', 'Zr_OH_4', 'ZrSi2', 'ZrS2', 'ZrO_NO3_2_2H2O', 'ZrO_CH3COO_2', 'ZrOCl2_8H2O', 'ZrO2', 'ZrN', and 'ZrI4'.

The right panel shows a list of files and folders. The columns are 'FILE NAME' and 'PATH'. The files listed are:

| FILE NAME | PATH |
|---|--|
| <input checked="" type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.system.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.user.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> README.csv | //SPring-8/BL14B2/Standard K_stabilized_ZrO2_ |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419.dat | //SPring-8/BL14B2/Standard |

Below the file list, there is a table of metadata for the selected file:

| | |
|-------------------------------------|---|
| @subject@correspondance@affiliation | JASRI |
| @subject@create_time | 2019-03-27 21:23:47 |
| @subject@disk_name | Standard |
| @subject@facility | SPring-8 |
| @subject@pid | spring8.32caaefe-e665-494b-e |
| @subject@proposal_number | 2014S0000 |
| @subject@register_name | /SPring-8/BL14B2/Standard/Zr/K/311/s K_stabilized_ZrO2_YSZ__Si3' |
| @subject@representative@username | 0007719 |

Directory structure with explore style

Web portal (Accessible data for user)

Full-text search



The screenshot displays the 'Experimental Data Transfer System' web portal. At the top, the header includes the system name, a user ID '0000664', and a 'LOGOUT' button. Below the header, there is a search bar containing the text 'Zr', a 'Search under folder' button, a dropdown menu set to 'your proposal', and a 'DOWNLOAD CHECKED ITEMS' button. The main content area is split into two panels. The left panel shows a hierarchical directory structure in an 'explore' style, starting from 'root' and navigating through 'SPring-8', 'BL14B2', 'Standard', 'Zr', 'K', and '311'. The folder 'stabilized_ZrO2_YSZ_' is highlighted in blue. The right panel shows a table of search results with columns for 'FILE NAME' and 'PATH'. The first row is checked, showing the file 'Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.json' with its full path. Below the table, a metadata section lists various attributes such as '@subject@correspondance@affiliation', '@subject@create_time', and '@subject@proposal_number' with their corresponding values.

| FILE NAME | PATH |
|---|----------------------------|
| <input checked="" type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.system.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.user.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> README.csv | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419.dat | //SPring-8/BL14B2/Standard |

| | |
|-------------------------------------|--------------------------------------|
| @subject@correspondance@affiliation | JASRI |
| @subject@create_time | 2019-03-27 21:23:47 |
| @subject@disk_name | Standard |
| @subject@facility | SPring-8 |
| @subject@pid | spring8.32caaefe-e665-494b-e |
| @subject@proposal_number | 2014S0000 |
| @subject@register_name | /SPring-8/BL14B2/Standard/Zr/K/311/s |
| @subject@representative@username | 0007719 |

Directory structure with explore style

Web portal (Accessible data for user)

Full-text search



Experimental Data Transfer System UID: 0000664 [LOGOUT](#)

your proposal

- root
 - SPring-8
 - BL14B2
 - Standard
 - Zr
 - K
 - 311
 - stabilized_ZrO2_YSZ_**
 - stabilized_ZrO2_MSZ_
 - stabilized_ZrO2_CSZ_
 - approx_ZrSiO4
 - Zr_SO4_2_4H2O
 - Zr_OH_4
 - ZrSi2
 - ZrS2
 - ZrO_NO3_2_2H2O
 - ZrO_CH3COO_2
 - ZrOCI2_8H2O
 - ZrO2
 - ZrN
 - ZrI4

| FILE NAME | PATH |
|---|---|
| <input checked="" type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.system.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.user.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> README.csv | //SPring-8/BL14B2/Standard/K_stabilized_ZrO2_ |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419.dat | //SPring-8/BL14B2/Standard |

| | |
|-------------------------------------|--------------------------------------|
| @subject@correspondance@affiliation | JASRI |
| @subject@create_time | 2019-03-27 21:22:17 |
| @subject@disk_name | Standard |
| @subject@facility | SPring-8 |
| @subject@pid | spring8.32caae |
| @subject@proposal_number | 2014S0000 |
| @subject@register_name | /SPring-8/BL14B2/Standard/Zr/K/311/s |
| @subject@representative@username | 0007719 |

Directory structure with explore style

Metadata view for selected file

Web portal (Accessible data for user)

Full-text search

Experimental Data Transfer System UID: 0000664 [LOGOUT](#)

[Search under folder](#) your proposal [DOWNLOAD CHECKED ITEMS](#)

Download file via zip

- root
 - SPring-8
 - BL14B2
 - Standard
 - Zr
 - K
 - 311
 - stabilized_ZrO2_YSZ_
 - stabilized_ZrO2_MSZ_
 - stabilized_ZrO2_CSZ_
 - approx_ZrSiO4
 - Zr_SO4_2_4H2O
 - Zr_OH_4
 - ZrSi2
 - ZrS2
 - ZrO_NO3_2_2H2O
 - ZrO_CH3COO_2
 - ZrOCI2_8H2O
 - ZrO2
 - ZrN
 - ZrI4

| FILE NAME | PATH |
|---|----------------------------|
| <input checked="" type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.system.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419_fe.user.json | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> README.csv | //SPring-8/BL14B2/Standard |
| <input type="checkbox"/> Zr-K_stabilized_ZrO2_YSZ__Si311_50ms_170419.dat | //SPring-8/BL14B2/Standard |

Directory structure with explore style

Metadata view for selected file

| | |
|-------------------------------------|--------------------------------------|
| @subject@correspondance@affiliation | JASRI |
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| @subject@facility | SPring-8 |
| @subject@pid | spring8.32caae |
| @subject@proposal_number | 2014S0000 |
| @subject@register_name | /SPring-8/BL14B2/Standard/Zr/K/311/s |
| @subject@representative@username | 0007719 |

Thumbnail for dataset

SPring-8 Experimental Data Transfer System

UID: 0000664 LOGOUT

Search under folder your proposal DOWNLOAD CHECKED ITEMS

root

- SPring-8
 - BL14B2
 - Standard
 - Zr
 - K
 - 311
 - 111
 - Zn
 - V
 - Ti
 - Sn
 - Sb
 - Ru
 - Rh
 - Pt
 - Pd
 - Ni
 - Nd
 - Nb
 - Mo
 - Mn
 - La
 - In
 - Fe
 - Cu

| DL | FILE NAME |
|--------------------------|----------------------|
| <input type="checkbox"/> | stabilized_ZrO2_YSZ_ |
| <input type="checkbox"/> | stabilized_ZrO2_MSZ_ |
| <input type="checkbox"/> | stabilized_ZrO2_CSZ_ |
| <input type="checkbox"/> | approx_ZrSiO4 |
| <input type="checkbox"/> | Zr_SO4_2_4H2O |
| <input type="checkbox"/> | Zr_OH_4 |
| <input type="checkbox"/> | ZrSi2 |
| <input type="checkbox"/> | ZrS2 |
| <input type="checkbox"/> | ZrO_NO3_2_2H2O |
| <input type="checkbox"/> | ZrO_CH3COO_2 |
| <input type="checkbox"/> | ZrOCl2_8H2O |
| <input type="checkbox"/> | ZrO2 |
| <input type="checkbox"/> | Zr-N |

Zr-K_stabilized_ZrO2_YSZ_Si111_50ms_170602

μt

Energy [eV]

- Thumbnail can be attached to dataset
- monitored in Web with metadata items

Thumbnail for dataset

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- Thumbnail can be attached to dataset
- monitored in Web with metadata items

Example:
XAFS spectrum plot
→ Useful for users

Summary: BENTEN features list

- Easy-to-use and generic experimental data transfer at SPring-8
 - Unified REST API for all the functions

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Summary: BENTEN features list

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 - Unified REST API for all the functions
- Implement authentication
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- Flexible metadata management
 - Metadata can be easily described in separate files (JSON or YAML format)
 - Existing data format in the measurements can be used as they are
 - Full-text search for flexible data access using Elasticsearch

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 - For restricted data access / Open data access
 - Use proposal number to derive range of data sharing
- Flexible metadata management
 - Metadata can be easily described in separate files (JSON or YAML format)
 - Existing data format in the measurements can be used as they are
 - Full-text search for flexible data access using Elasticsearch
- Data management
 - Data life cycle
 - Creation, Update, Open/Closed access, Delete
 - Clarify Contact name for Open data

Current status and Future plan

- Operation of BENTEN at SPring-8 since March, 2019
 - Provided data access thorough the Internet
 - Open data for XAFS standard sample
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 - Remote data access for CT (Computed Tomography) image

➔ Will start within a year