HELMHOLTZ METADATA COLLABORATION

HZB Helmholtz Zentrum Berlin

FAIR meets EMIL

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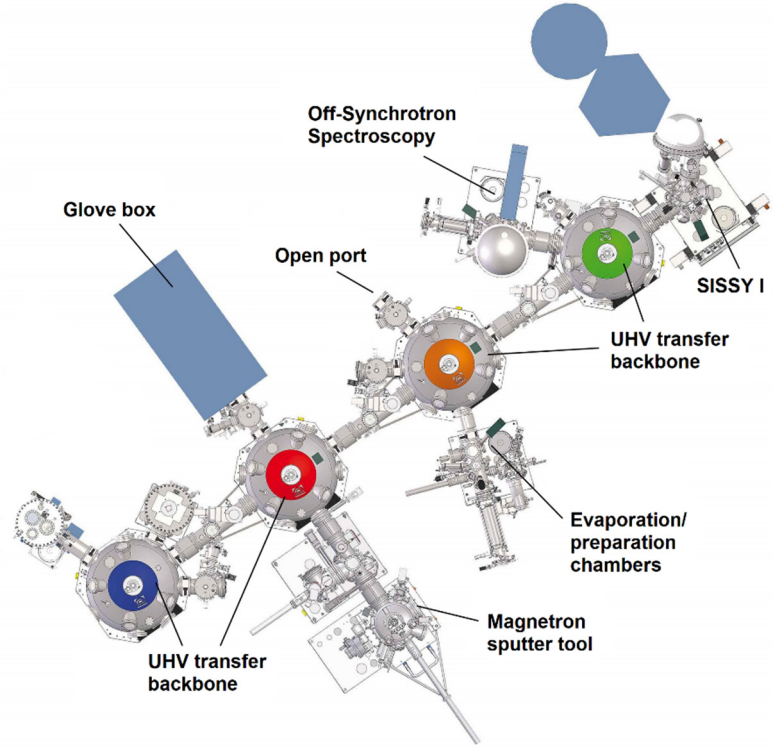
Nico Greve // Rolf Krahl // Simone Vadilonga // Regan Wilks // Oonagh Mannix.

Helmholtz-Zentrum Berlin für Materialien und Energie

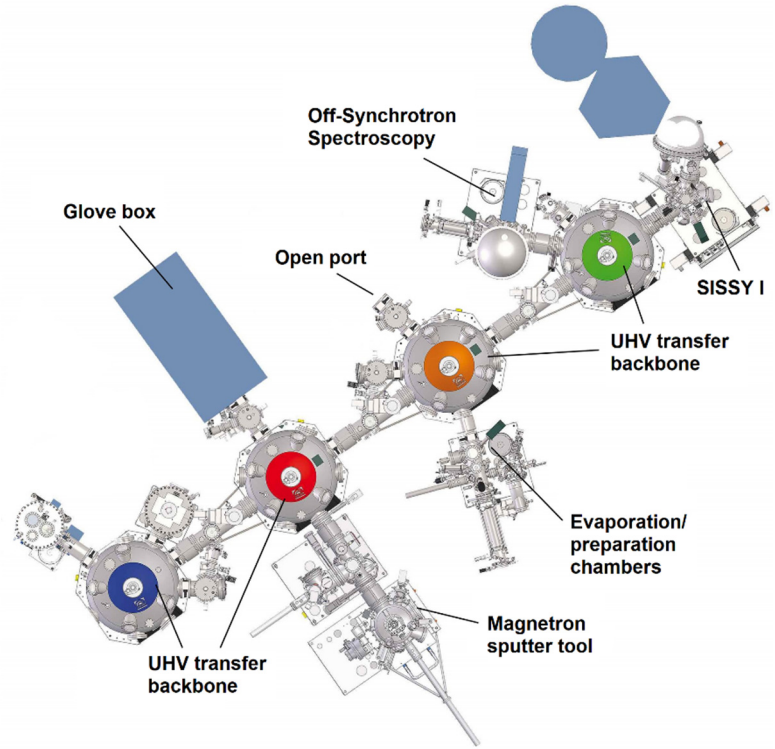
EMIL - Energy Material In-Situ Laboratory Berlin



Applying FAIR criteria on end station during commissioning phase:

- SISSY@EMIL infrastructure
- Reusability
- Interoperability
- Accessibility
- Findability
- Provided workflows

EMIL - Energy Material In-Situ Laboratory Berlin



Complex Infrastructure:

Fully-automated vacuum transfer system connecting

- Sample processing (sputtering, thin films…)
- Off-Synchrotron analysing systems

Synchrotron end station SISSY I

- BlueSky Control System
  ⇨ Details: *FRBR03, Fr, William Smith: Status of BlueSky Deployment at BESSY II*

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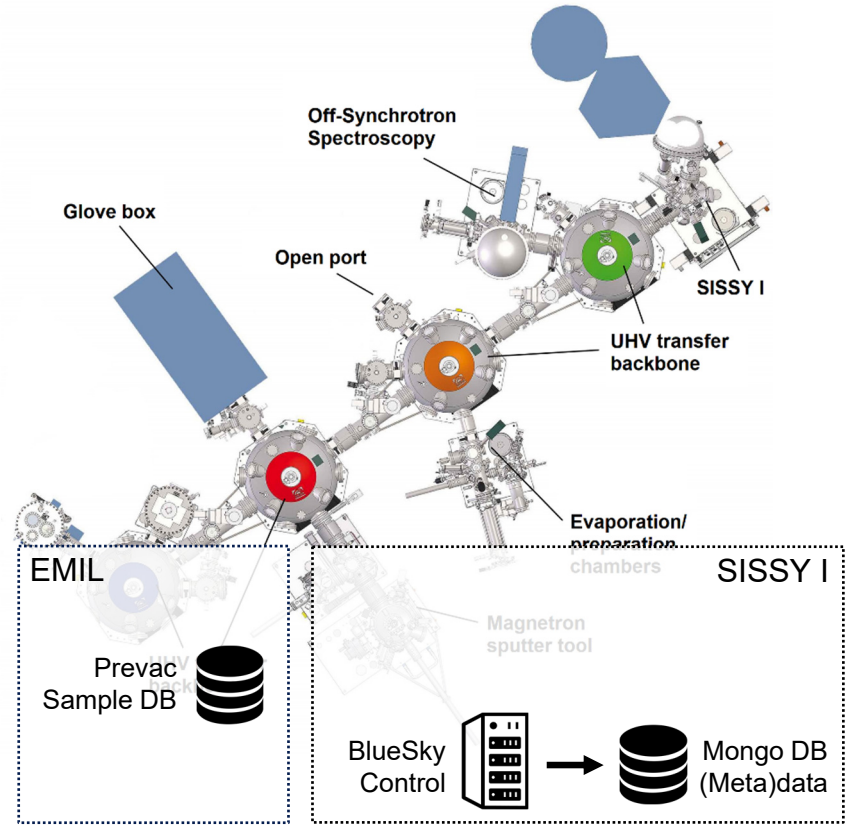

Complex Infrastructure:

Fully-automated vacuum transfer system connecting

- Sample processing (sputtering, thin films…)
- Off-Synchrotron analysing systems
- **Prevac Sample Database**

Synchrotron end station SISSY I

- BlueSky Control System
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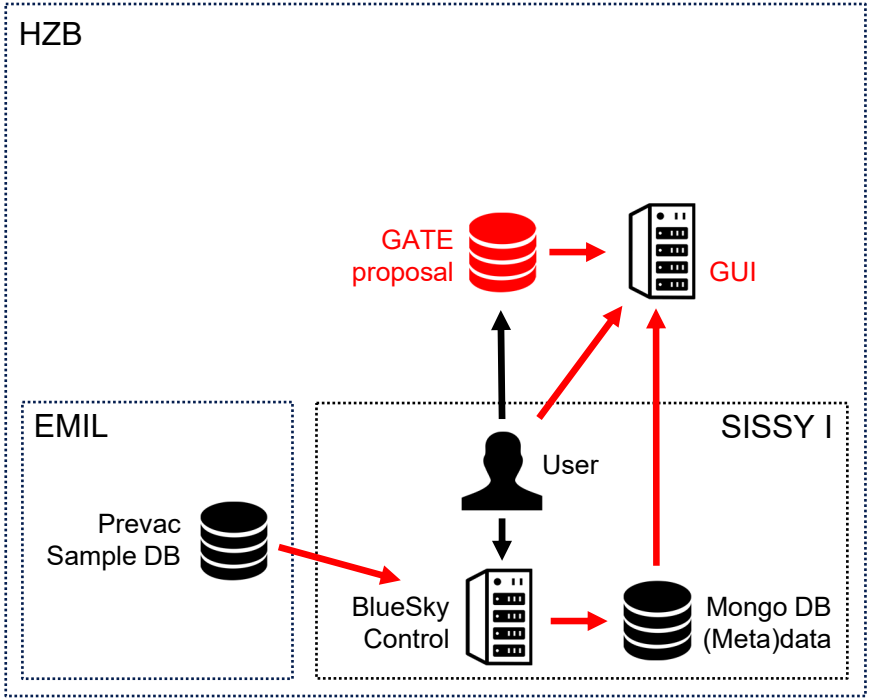
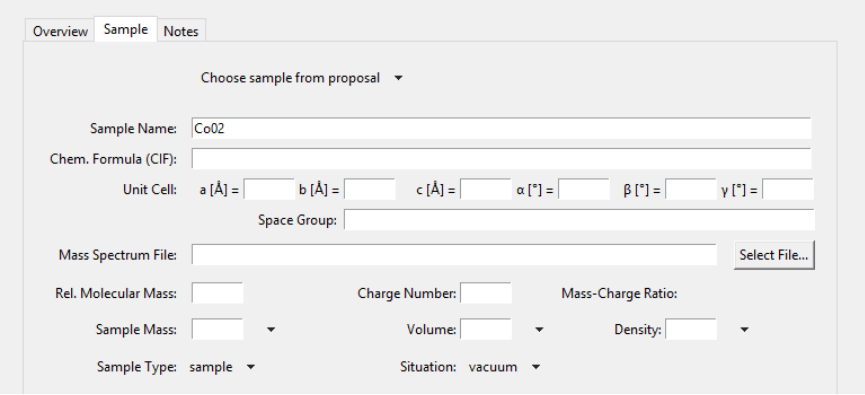
- **Mongo Database with measurement (meta)data**

Reusability – Richness of Metadata

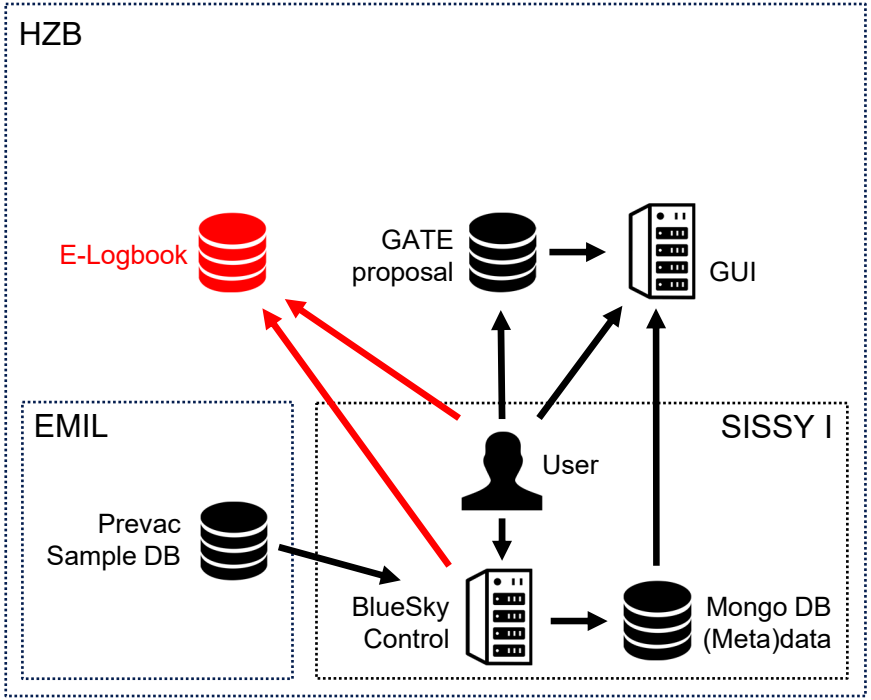


Mainly measures on instrument level:

- Sample information
  - Pseudo-sample axis in control software (BlueSky GUI)
  - Readout of Prevac sample DB
  - GUI to enter sample metadata
    (separate from instrument control to minimize impact)
  - Readout of proposal sample data (currently only pdf)



Reusability – Richness of Metadata



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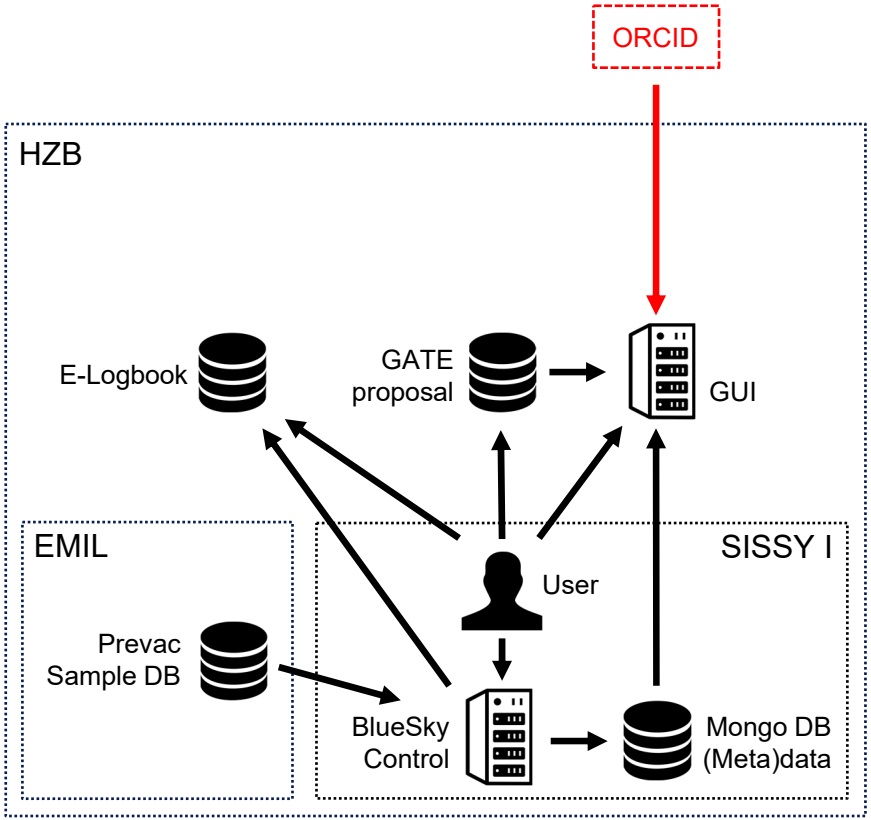
- E-Logbook
  - User: notes, conclusions or classifications
  - Instrument: Selected parameters

Reusability – Richness of Metadata



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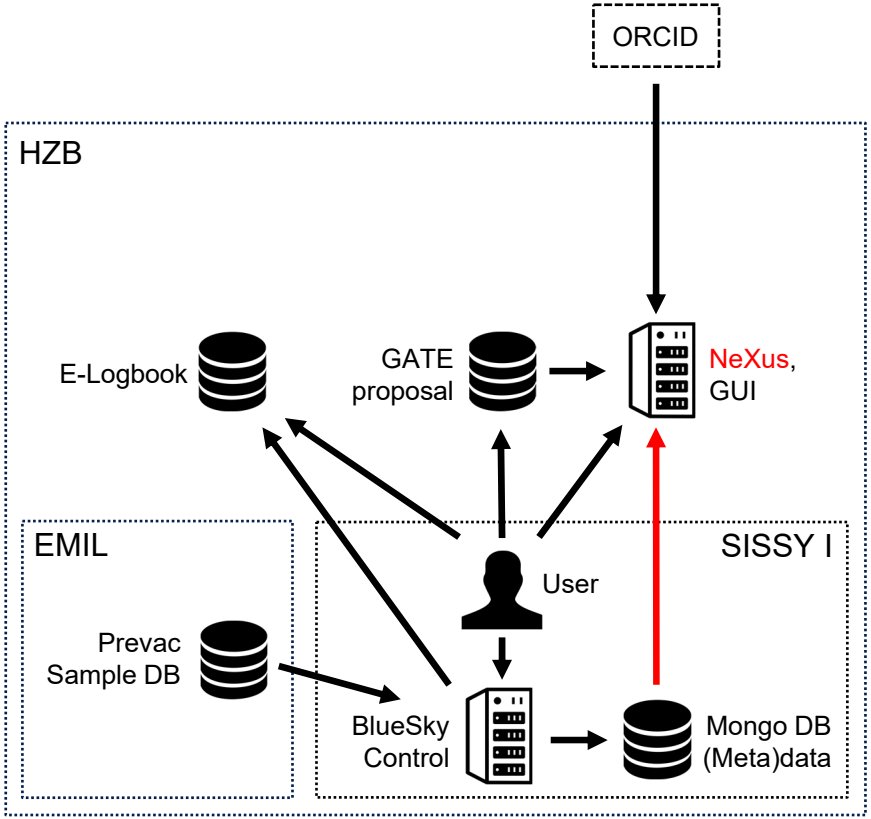
- E-Logbook
  - User: notes, conclusions or classifications
  - Instrument: Selected parameters
- PIDs (not on instrument level)

  To make important information unambigious
  - Instrument PIDs
  - ORCIDs

Interoperability



Converte database to NeXus

- Standard in x-ray and neutron science
- NeXus Definition Language defines nomenclature and arrangement of (meta)data
- HDF5 file format is suitable for high-performance data processing
- Supported by capable software (e.g. Dawn)

Structure:

ENTRY: (required) NXentry

@entry: (required) NX_CHAR

NeXus convention is to use “entry1”, “entry2”, … for analysis software to locate each entry.

title: (required) NX_CHAR

start_time: (required) NX_DATE_TIME

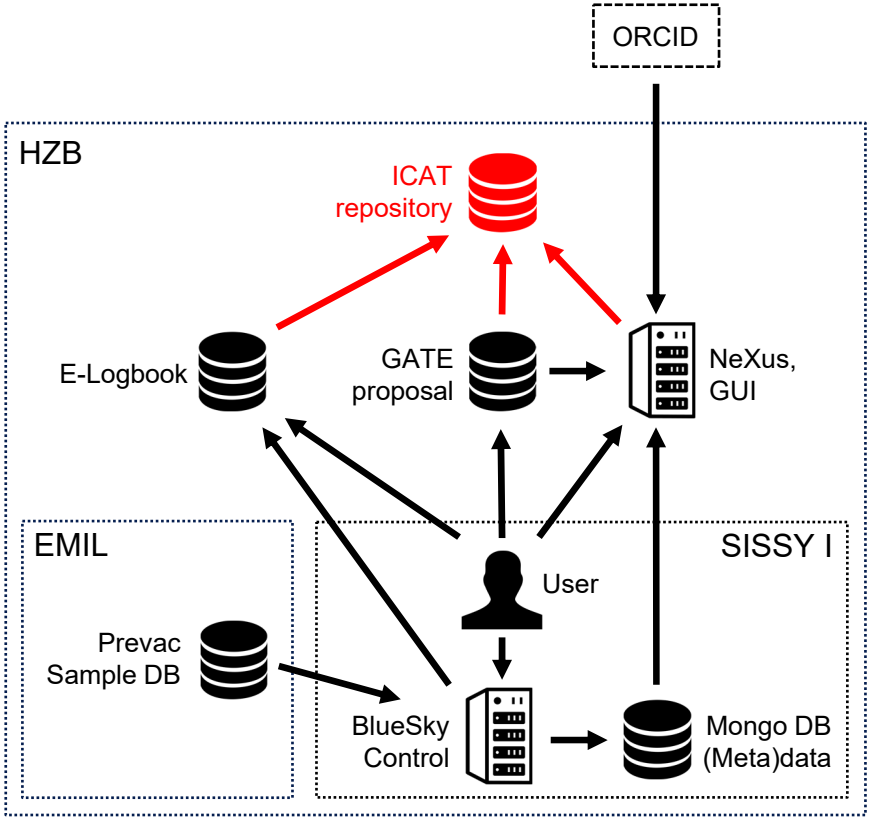
definition: (required) NX_CHAR

Official NeXus NXDL schema to which this file conforms

Obligatory value: `NXxas`

INSTRUMENT: (required) NXinstrument

Accessibility



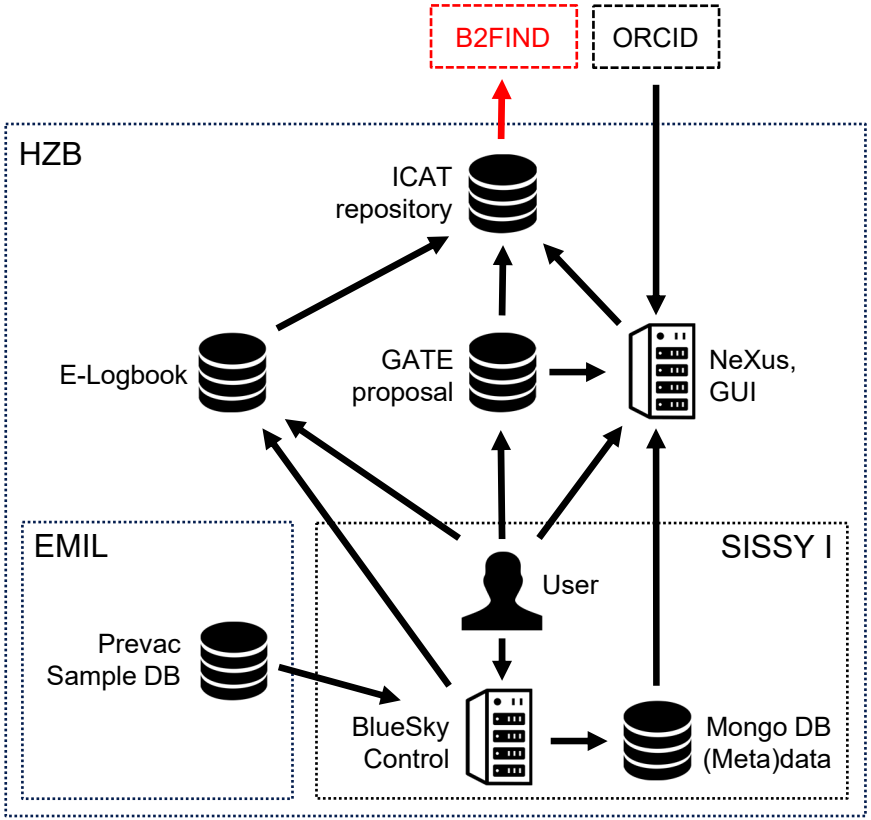
Connection to HZB repository:

- Instance of ICAT used by other facilities (e.g. ISIS, Diamond Light Source, ESRF)
- (Meta)data is accessible through HTTP
- Authentication System
- Tape library may hinder machines

HZB / *Investigation*

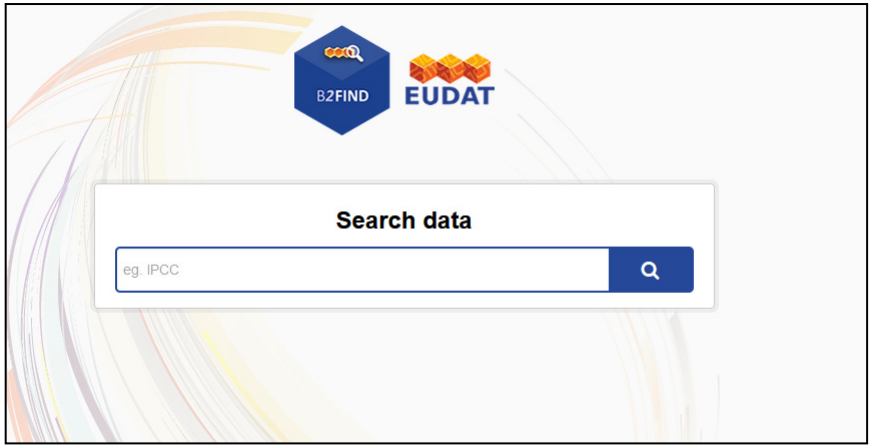
Investigation	Title	Instrument
Containing...	Containing...	Containing...
gate1:16204712-EF-1.1-N	Crystal Structure and Diffuse Scattering in th...	E2 - Flat-Cone Diffractometer
gate1:16203966-EF-1.1-N	Test measurement for check the quality of a ...	E2 - Flat-Cone Diffractometer
gate1:16204038-ST-1.1-N	Ising quantum criticality in transverse fields i...	E2 - Flat-Cone Diffractometer
gate1:16204081-ST-1.1-N	Analysis of the wide-angle neutron scatterin...	E9 - Fine Resolution Powder D
gate1:16204074-ST-1.1-N	Stability of magnetic order in partially frustrat...	E2 - Flat-Cone Diffractometer
gate1:16204440-ST-1.1-N	Testing the Order-by-Disorder hypothesis in ...	E2 - Flat-Cone Diffractometer
gate1:16103849-ST-1.1-N	Magnetic order in a J=0 perovskite iridate	E2 - Flat-Cone Diffractometer
gate1:16204257-EF-1.1-N	Magnetic Diffuse Scattering of two New Rare...	E2 - Flat-Cone Diffractometer
gate1:16103893-ST-1.1-N	Magnetic order in new low dimensional Ising ...	E2 - Flat-Cone Diffractometer
gate1:16103708-EF-1.1-N	Determination of oxygen sites in the crystal l...	E9 - Fine Resolution Powder D
gate1:16103495-ST-1.1-N	Phase diagram of potassium nitrate nanopar...	E9 - Fine Resolution Powder D
gate1:16103774-ST-1.1-N	Change of magnetic order by non-magnetic ...	E2 - Flat-Cone Diffractometer

Findability

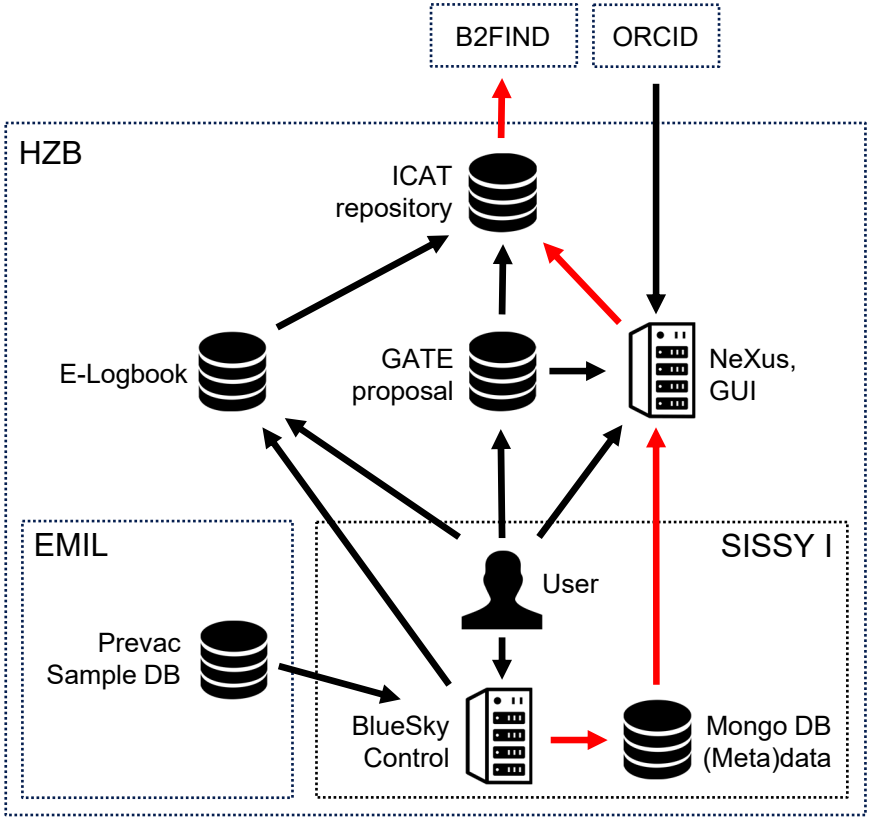


Connection to high-level services:

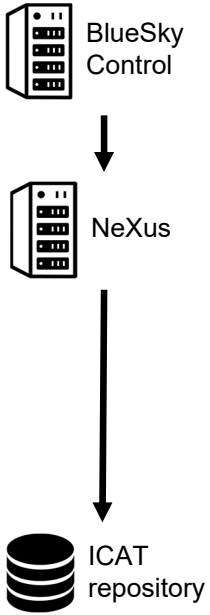
- Manual assignment of PIDs for data publications
- Automatic assignment of PID for raw data files is work in progress
- Harmonization of metadata schema with regard to B2FIND



Workflows – User‘s Point of View



Automatic



☺ **Workload**
😐 **Data accuracy**

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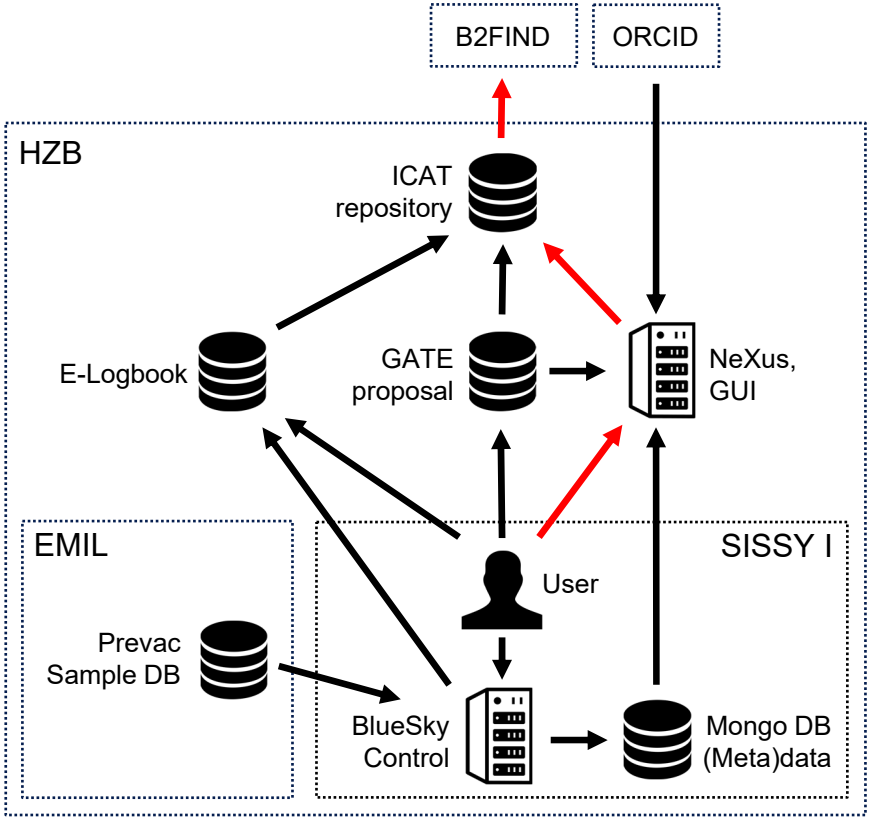

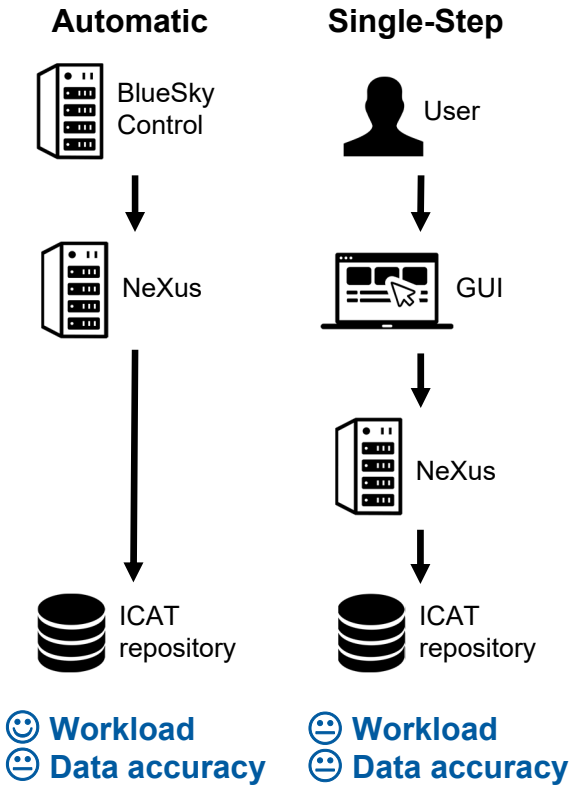

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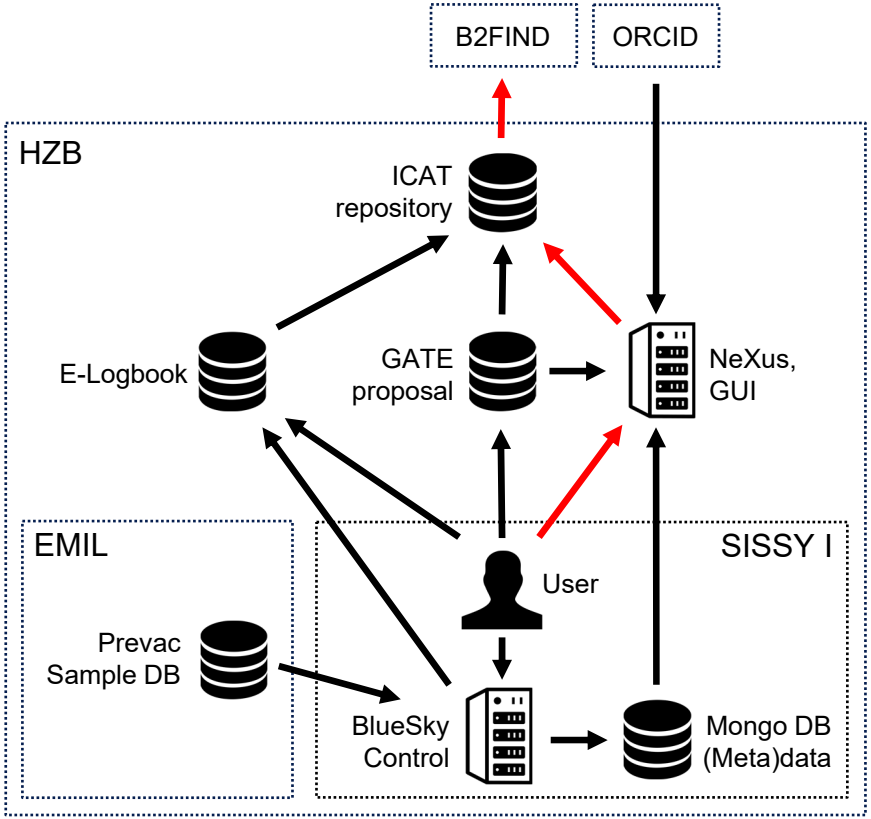

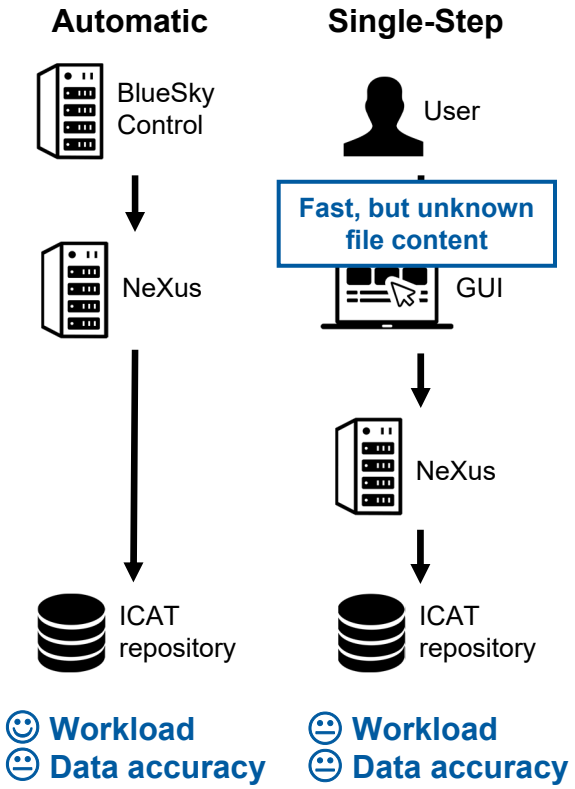

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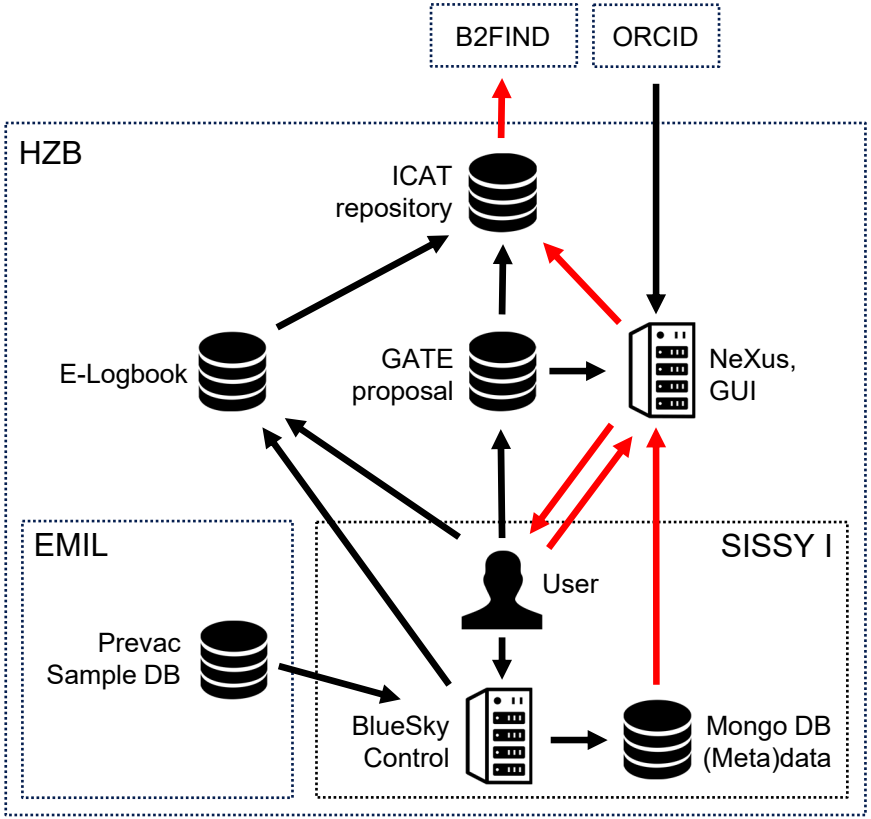

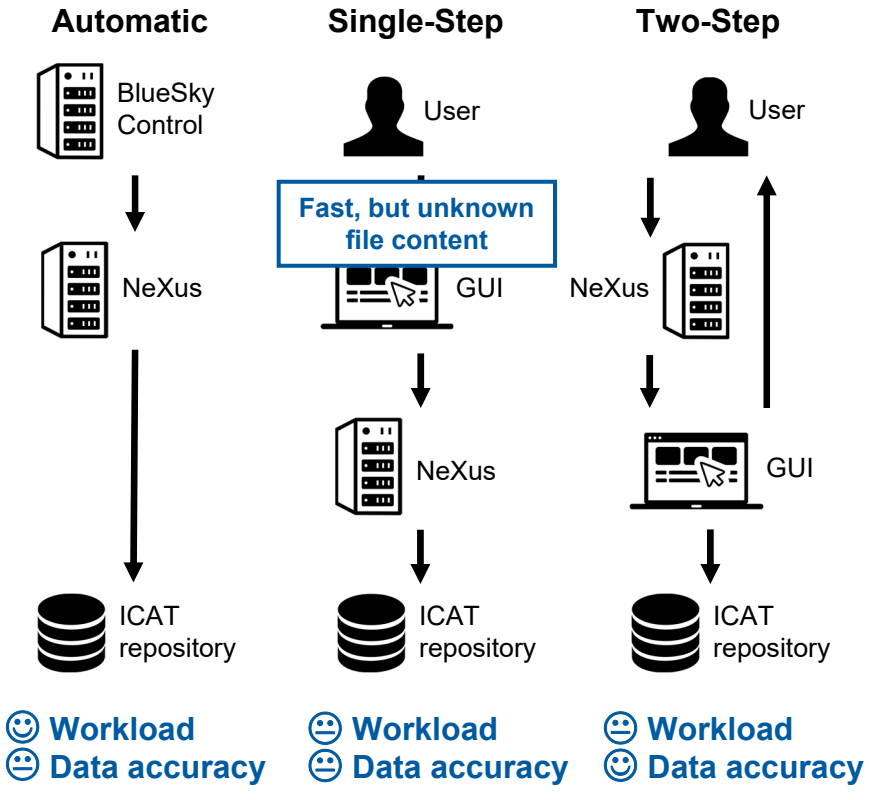

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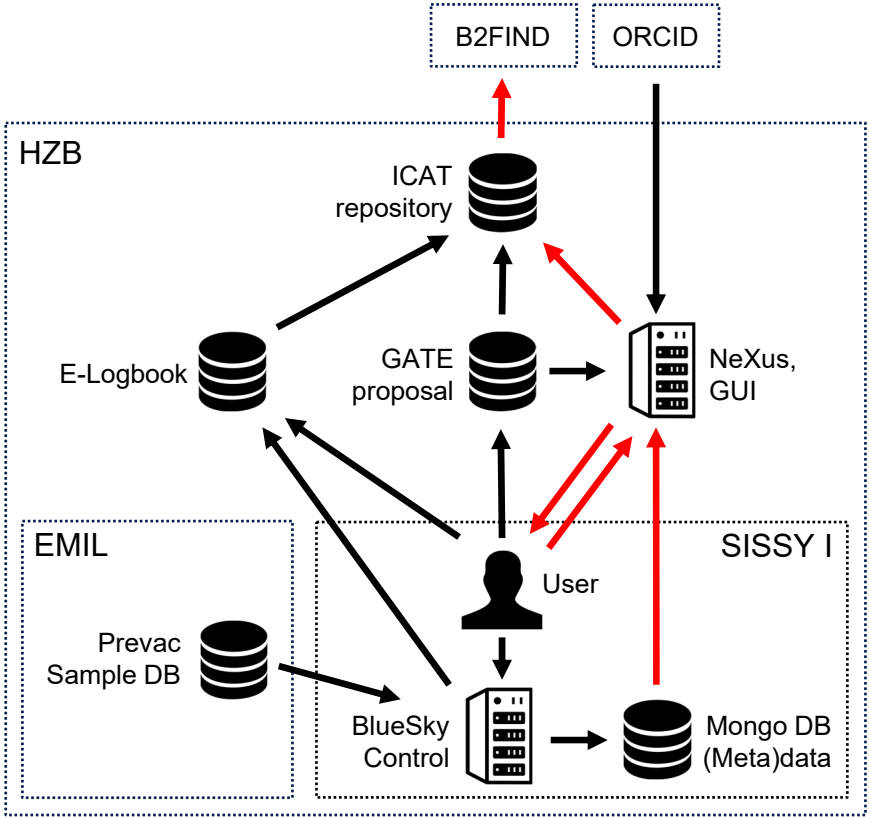
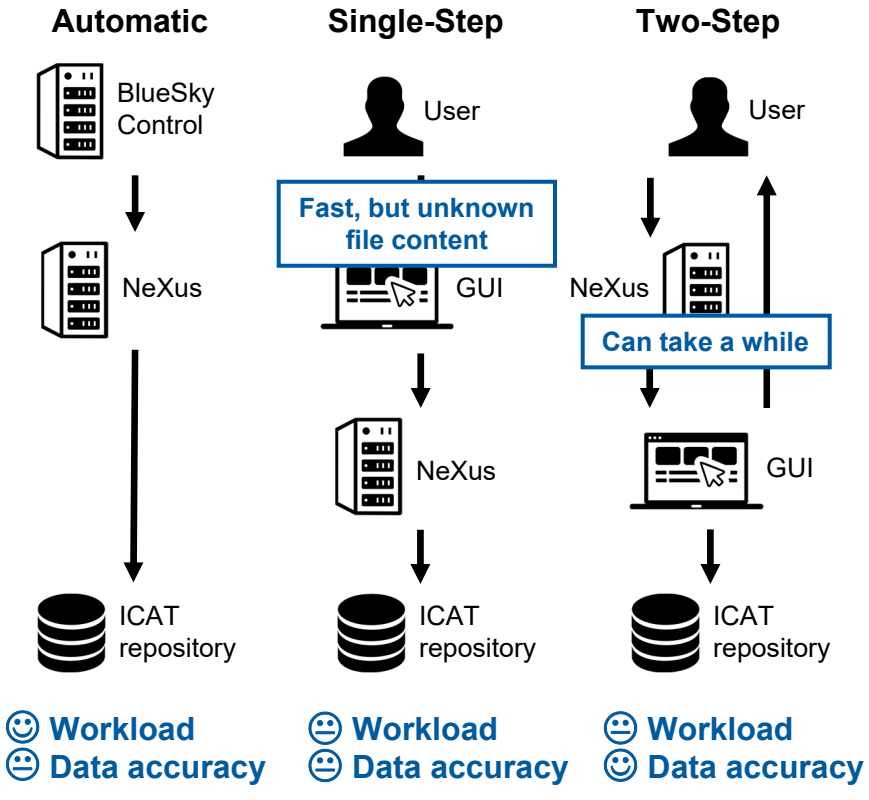
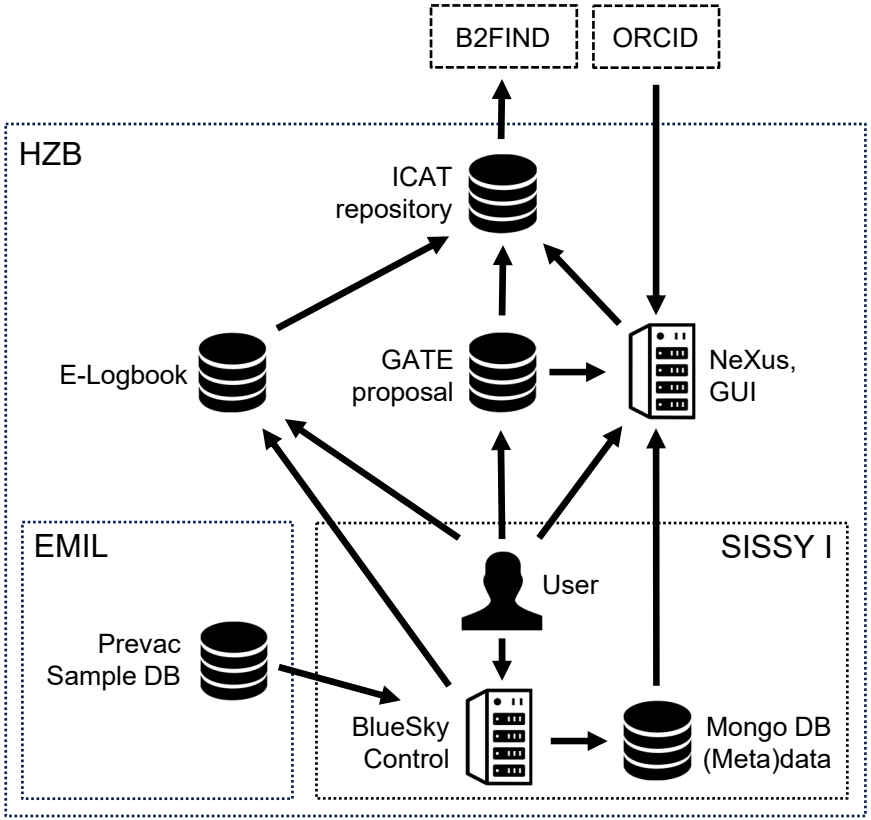




Summary



Reusability:

- Mainly on instrument level
- Dynamic process of mutually induced steps

Interoperability:

- NeXus writing routine

Accessibility:

- Connection to repository
- Tape library may hinder machines

Findability:

- Automatic assignment of PIDs
- Connection to high-level services (e.g. B2FIND)

Meet essential criteria of FAIR Maturity Model soon