

SciCat for P10 DESY

Proposed metadata schema draft

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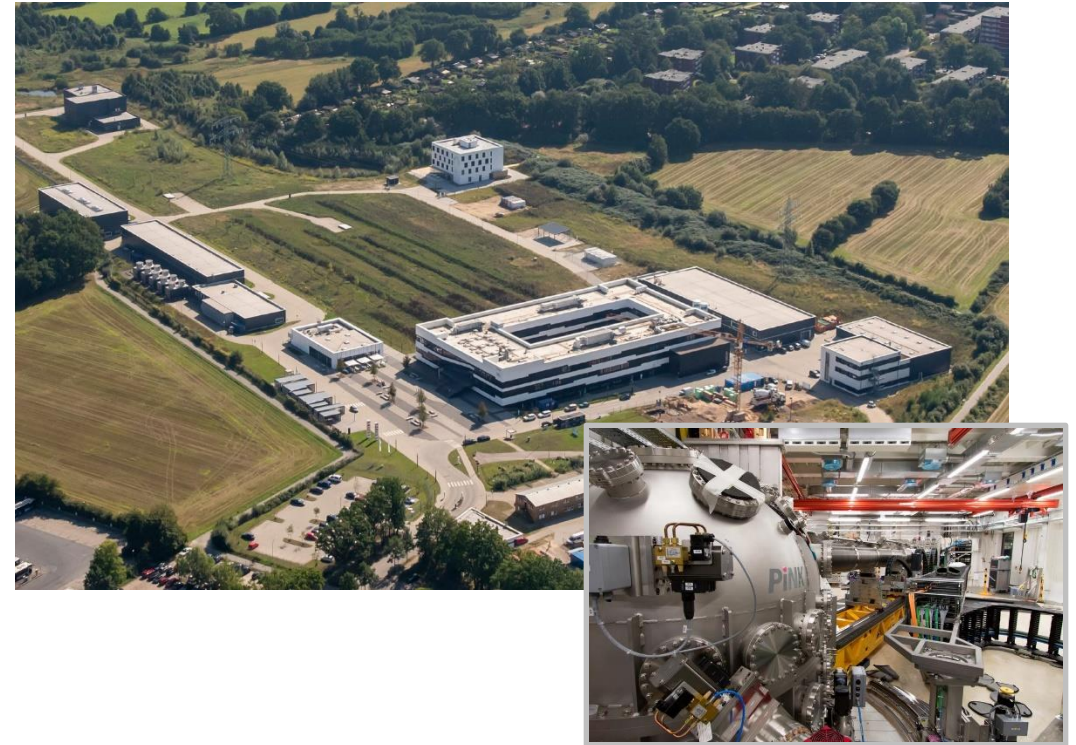
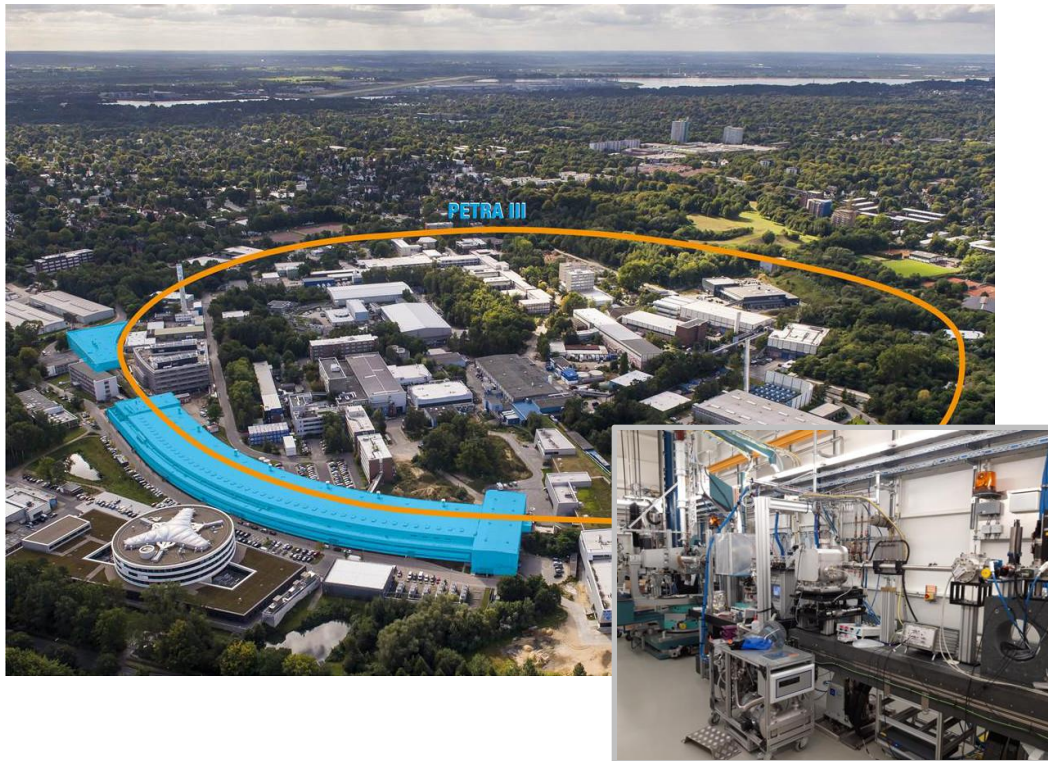
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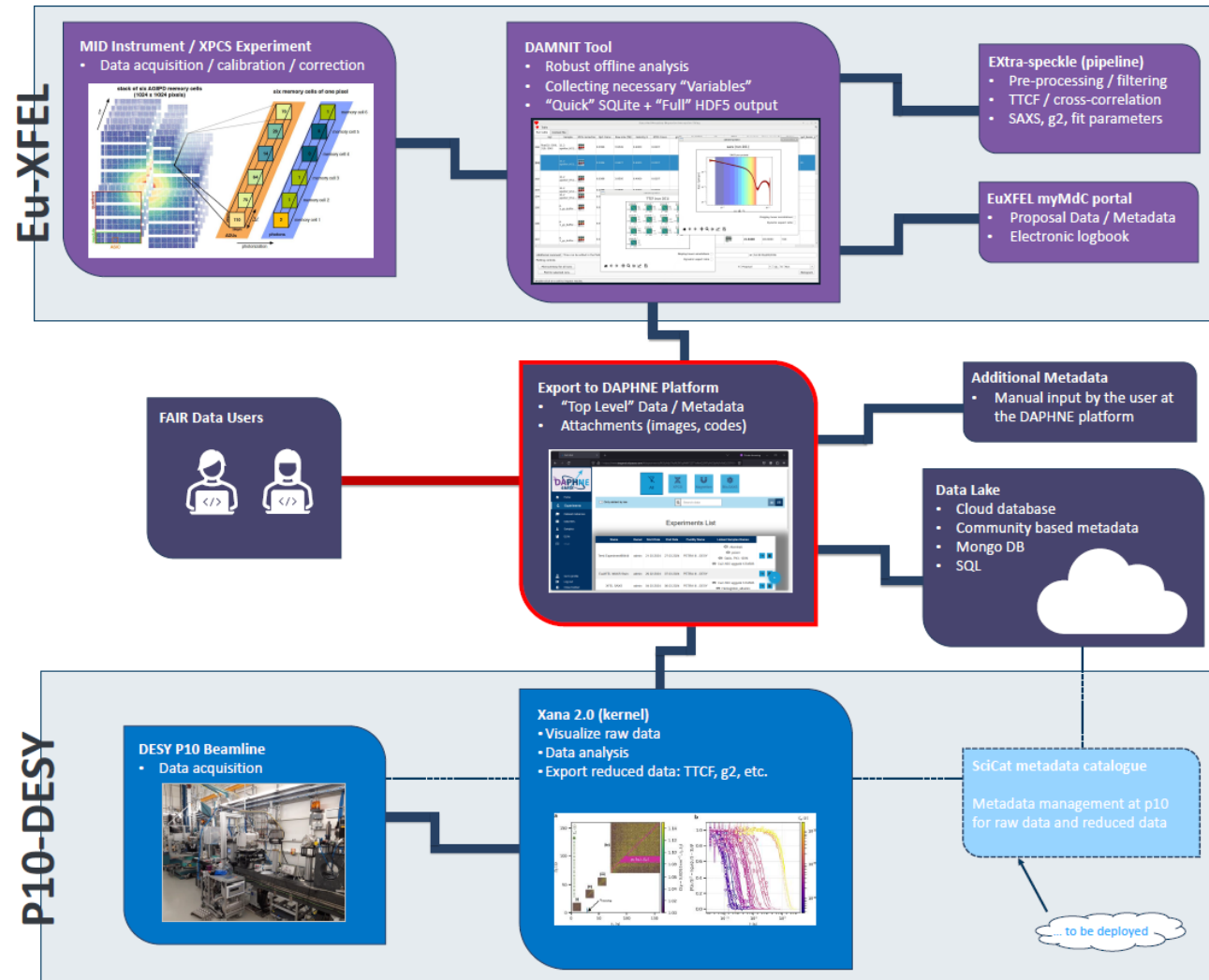
Experimental Facilities

P10 beamline @ Petra III



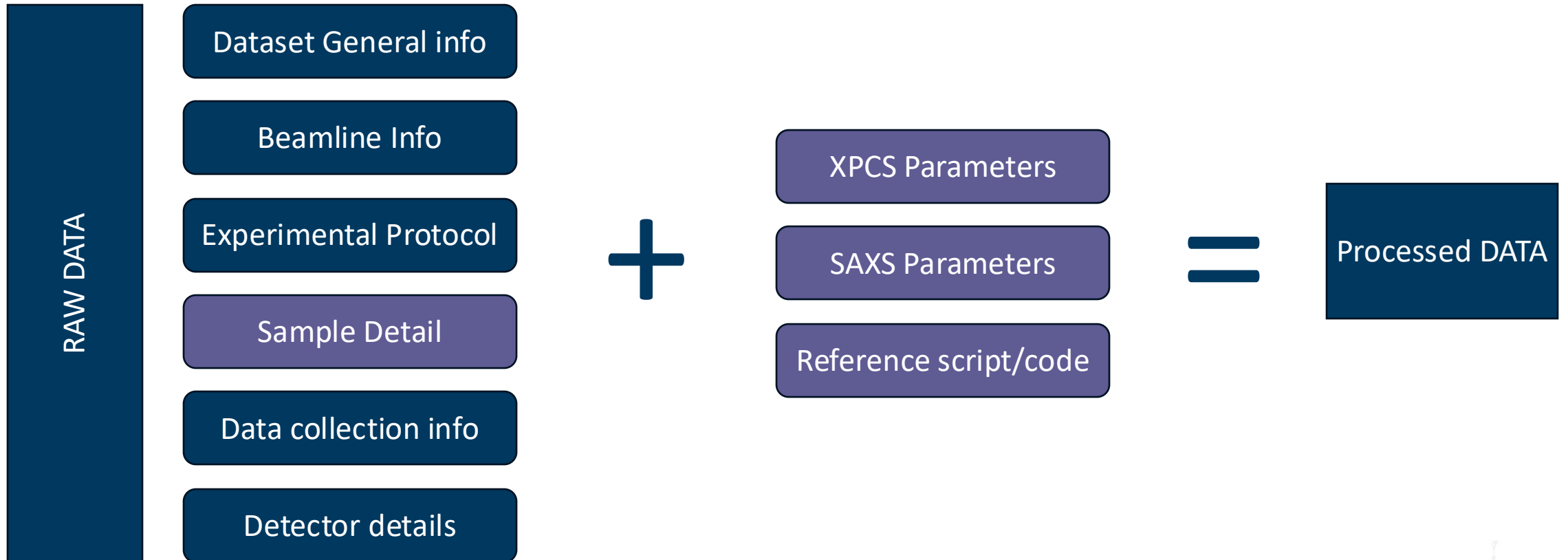
MID beamline @ EuXFEL

General plan



- Establishing the communication pipeline between DAPHNE platform and data storage of European XFEL / DESY facilities
- Possibility to access facility data for the FAIR Data Users
- Providing computational resources for FAIR Data User
- SciCat connection (internal or external)

SciCat for P10-DESY



Raw Data Schema



Dataset General info

- Dataset Title: Raw SAXS/XPCS Data from [Sample Name] at DESY P10 Beamline
- Date of Dataset Creation: YYYY-MM-DD
- Dataset Description:
 - **Contains raw data from SAXS and XPCS experiments performed on [sample description], recorded at DESY P10 beamline. Includes detector output, beam settings, and initial data files.**
- Keywords:
 - **Raw SAXS data**
 - **Raw XPCS data**
 - **DESY P10**
 - **Coherent X-rays**
 - **Synchrotron**
 - **[Sample-specific keywords]**
- Data Type:
 - **HDF5, TIFF, or other raw formats (based on the detector)**

Beamline info

- Beamline Name: P10, PETRA III, DESY
- Beamline ID:
- X-ray Energy: 8.54 keV (adjustable based on the experiment)
- Detector:
 - Eiger4M
 - Other detectors if applicable
- Beam Size: 100 x 100 μm^2 or (* has to be measured and stored)
- Beam Flux: 2×10^{12} ph/s (* measured once per beamtime)
- Sample-to-Detector Distance: Adjustable (e.g., 2 m, 3 m)
- Beam Attenuators: [Details of any attenuators used]

Experimental Protocol

- Experiment Type: SAXS/XPCS
- Temperature Range: Room temperature to 100°C (adjust as per experiment)
- Exposure Time per Frame: 0.001 - 1 s
- Transmission: 0.01 - 0.1
- Frames per Scan: 1500 frames

Sample Details

- Sample Names: [Sample 1, Sample 2]
- Sample Environment
- Sample Holder Details: Quartz capillaries or [other sample holder details]
- Sample Concentration
- Buffer Info

Raw Data Collection Information

- Data File Format:
 - HDF5 for raw data storage
 - TIFF/PNG for detector images
 - Log files in TXT or CSV format
- Raw Data Structure:
 - Folder structure for raw data, including file naming conventions (e.g., sample_name_frame_number.tiff or scan_number.h5)
 - Detector output files containing raw intensity data
- Data Acquisition Details:
 - Number of frames per scan: 1500 frames
 - Number of scans per dataset: [Number of scans]
 - Time per scan: [Exposure time per frame × number of frames]

Data Collection Instrument / Detector Info

- Detectors Used:
 - Eiger4M (for XPCS)
 - Pilatus 1M (for SAXS)
- Temperature-Controlled Stage (if used): Linkam stage (or other) with temperature details
- Motor Positions:
 - X
 - Y
 - Z

Processed Data Schema



Dataset General info

- SAXS Parameters:
 - Beamline Mask information
 - User Mask information
 - Scattering Vector Range: $q = 0.005$ to 0.2 nm^{-1}
 - Intensity units
- XPCS Parameters:
 - Frame averaging applied over [number of frames].
 - Correlation function $g^2(q, \tau)$.
 - Normalization of the intensity correlation function.
 - Relaxation times (τ).
 - Q-Range: 0.005 to 0.2 nm^{-1}
 - Delay Time Range: $10 \mu\text{s}$ to $10,000 \text{ s}$ (or experiment-specific)

Reference Scripts/Code

Reference Scripts/Code

- Python scripts for XPCS analysis
- ATSAS tools for SAXS analysis

Thanks