Metadata for X-ray reflectivity at P08/PETRA III

ORSO Annual Meeting 2023

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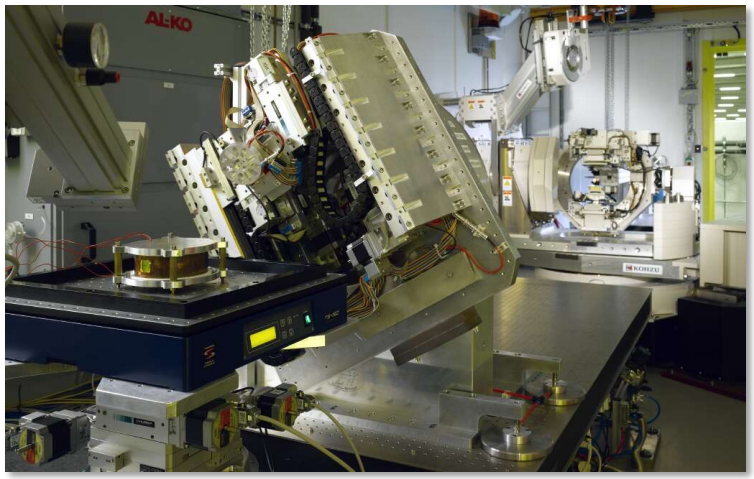
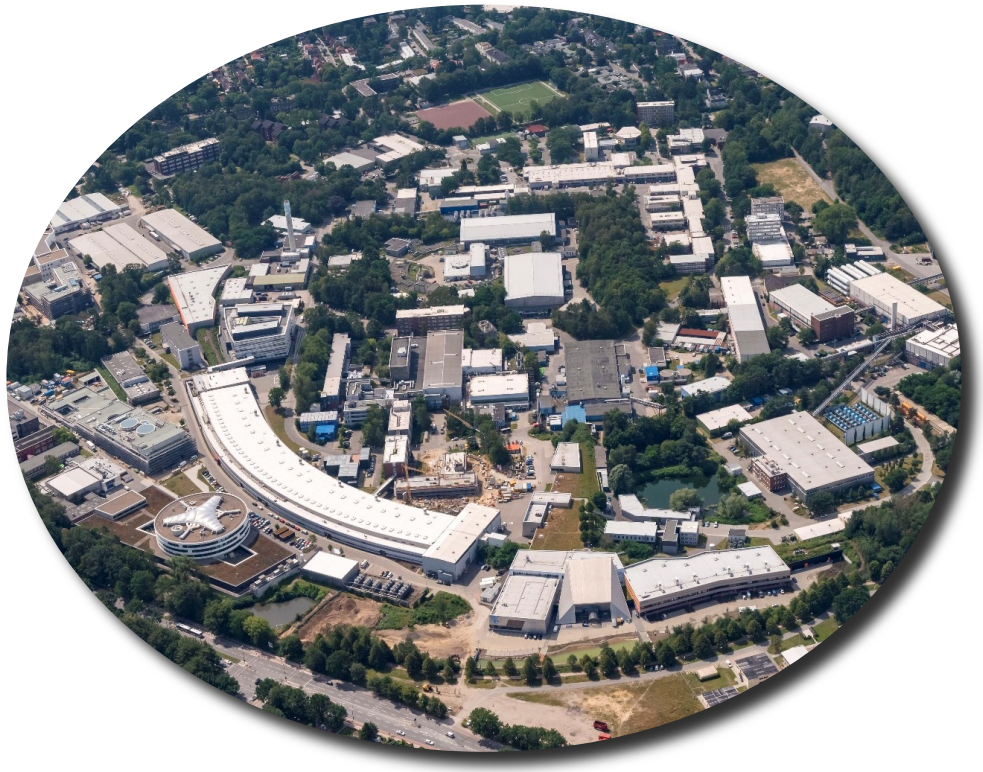
Beamline P08 / LISA

Experiments for X-ray reflectivity use case are performed at beamline P08/DESY at LISA diffractometer

- P08 as a test environment for DAPHNE solutions
- High resolution beamline, suited for XRR
- Liquid Interface Scattering Apparatus LISA:
  - Double Crystal Deflector (DCD)
  - Suitable of XRR experiments at liquid samples

LISA diffractometer





Managing Metadata Collection Workflow

Enabling re-use and repeatability of results, ideally searchable

Before experiment

Proposal
- *Proposal number (ID)*
- Science motivation
- Experiment concept
- Technique(s)
- Sample(s)
- Sample environment
- Instrumentation
- Science team

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Facility
- *Which facility?*
- Beam parameters
- Instrumentation
- Detectors

Digital Sample ID
- 'DOI for samples'
- (MX has sample QR codes)
- *Cross link to other consortia*

During experiment

Facility/machine logs
- *Experiment ID (directory)*
- Beam parameters
- Motor positions
- Instrument configuration
- Sample environment
- Detector calibration

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User record of experiment
- Instrumentation configuration
- Actual samples used
  - Ideally a digital sample ID
- Actual sample environment
- Changes to original plan
- What happened when
- Run log (data lookup table)
- Currently: Paper logbooks, google sheets, confluence, and more

Data can be 750 TB

After experiment

Analysis
- Data analysis steps
- Not all data is useful (runs)
- Intermediate data, code, scripts

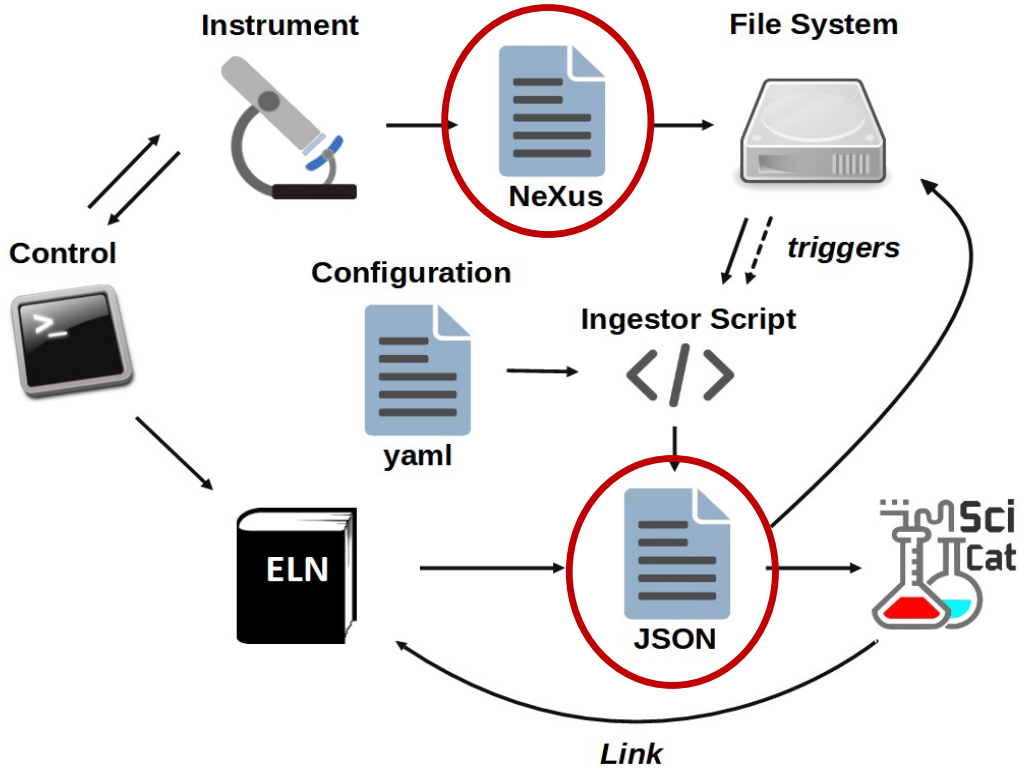
Publication
- Findable, searchable, descriptive
- *Citation, DOI reference*
- Sometimes data is deposited (PDB, CXIDB)
- May use a subset of data, or data from many experiments

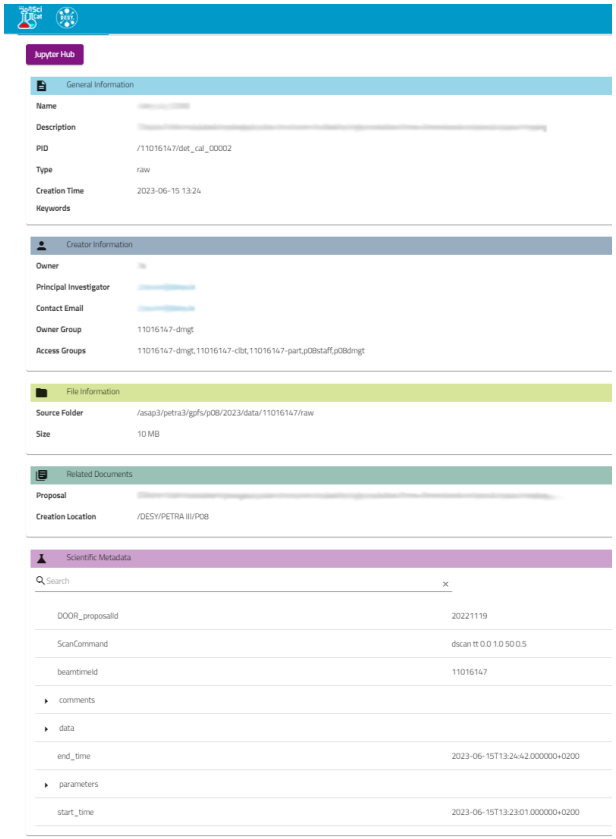
Re-use
- Check and verify results
- Improve the analysis
- Re-use code for new work
- Build on past data

Metadata Collection and Storage

Collection of metadata from the instrument and operator side

- ❑ NeXus files gather all metadata from the instrument
- ❑ Metadata catalogue SciCat for critical metadata
  - ➢ Increased findability of datasets





NeXus File Format – Instrument Representation

NeXus format for data at P08 in accordance with NeXus application definitions

- ❑ Instrument specification under NXInstrument
- ❑ Metadata (e.g. motor positions) from all beamline components
- ❑ Division of LISA in DCD, sample and detector metadata

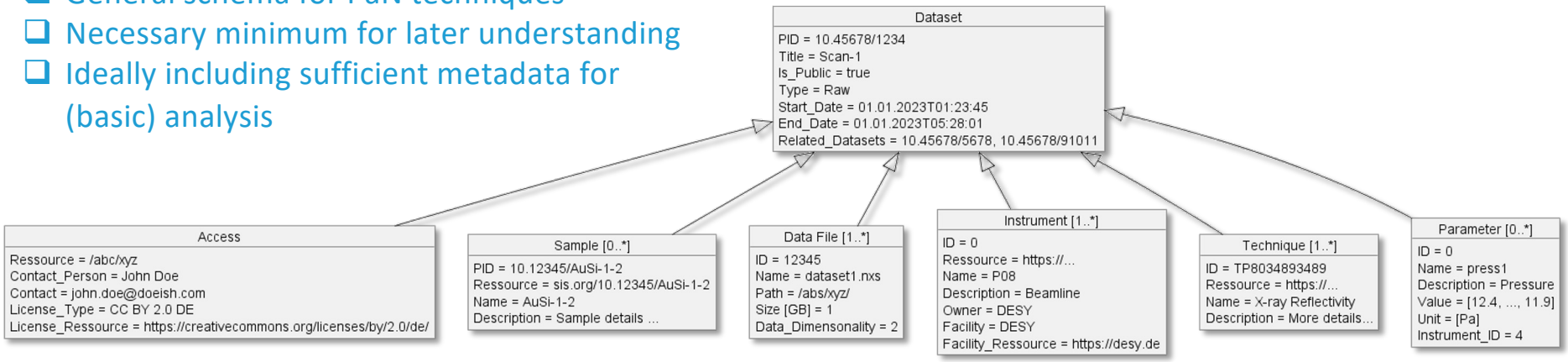
Name	Description	Type	Shape	Li
dppc_h2o_21c_00035.nxs		NXroot		
nexus_logs		NXcollection		
scan	"LISA beamtime"	NXentry		
apd		NXmonitor		
apd2		NXmonitor		
bpm1		NXmonitor		
bpm2		NXmonitor		
bpm3		NXmonitor		
bpm4		NXmonitor		
data		NXdata		
end_time	"2022-11-24T15:37:34.847219+0100"	string	scalar	
experiment_description	"PaNET01184"	string	scalar	
experiment_identifier	"11016627"	string	scalar	
instrument	"P08 High Resolution Diffraction Beamline"	NXinstrument		
ion1		NXmonitor		
ion2		NXmonitor		
ion_bl		NXmonitor		
lom_foil_vfc		NXmonitor		
program_name	"NexDaTaS"	string	scalar	
sample	"1,2-dipalmitoyl-sn-glycero-3-phosphatidylcholine"	NXsample		
start_time	"2022-11-24T15:37:05.125173+0100"	string	scalar	
title	"LISA beamtime"	string	scalar	

Name	Description	Type	Shape	Shape	Link
lisa_dcd		NXcollection			
abs	[3.99992]	float64	1		
lisa_dcd		NXtransformations			
alpha	1D data	float64	9		
m1rol	[-0.25]	float64	1		
m1th	[6.0532]	float64	1		
m1tra	[0]	float64	1		
m1tth	[12.1]	float64	1		
m2h	[53.7531]	float64	1		
m2rol	[-8.50912]	float64	1		
m2sh	[53.7531]	float64	1		External
m2th	[2.35903]	float64	1		
m2tra	[0]	float64	1		
m2tth	[-7.725]	float64	1		
mchi	1D data	float64	9		
trans2d	[0]	float64	1		
lisa_detector		NXdetector			
collection		NXcolleciton			
qpar	1D data	float64	9		
qx	1D data	float64	9		
qy	1D data	float64	9		
qz	1D data	float64	9		
lisa_detector_stage		NXtransformations			
beta	1D data	float64	9		
dalign	[0.0094]	float64	1		
dh	[0.9639]	float64	1		
dh_raw	[6.36459e+06]	float64	1		
drot	[0.100507]	float64	1		
dtth	1D data	float64	9		
stth	1D data	float64	9		
lisa_sample		NXcolleciton			

Minimum Viable Metadata Specification

Draft structure for minimal metadata schema by Philipp Jordt

- General schema for PaN techniques
- Necessary minimum for later understanding
- Ideally including sufficient metadata for (basic) analysis



Questions for discussion in ORSO

- Are there *necessary extensions* in the specific context of reflectometry?
- What is a suitable set of *required* metadata in reflectometry? In particular, what needs to be carried on to the reduced reflectivities for further analysis?

Summary

XRR use case at DESY/P08

- ❑ Workflows for the collection, curation and storage of metadata
- ❑ NeXus format with detailed instrument description with base classes
- ❑ Minimum metadata specification adaptable to reflectometry specifically

Acknowledgement
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