Workshop on Raw Diffraction Data Reuse:
“The Good, the Bad and the Challenging”

Handling big data at the European XFEL

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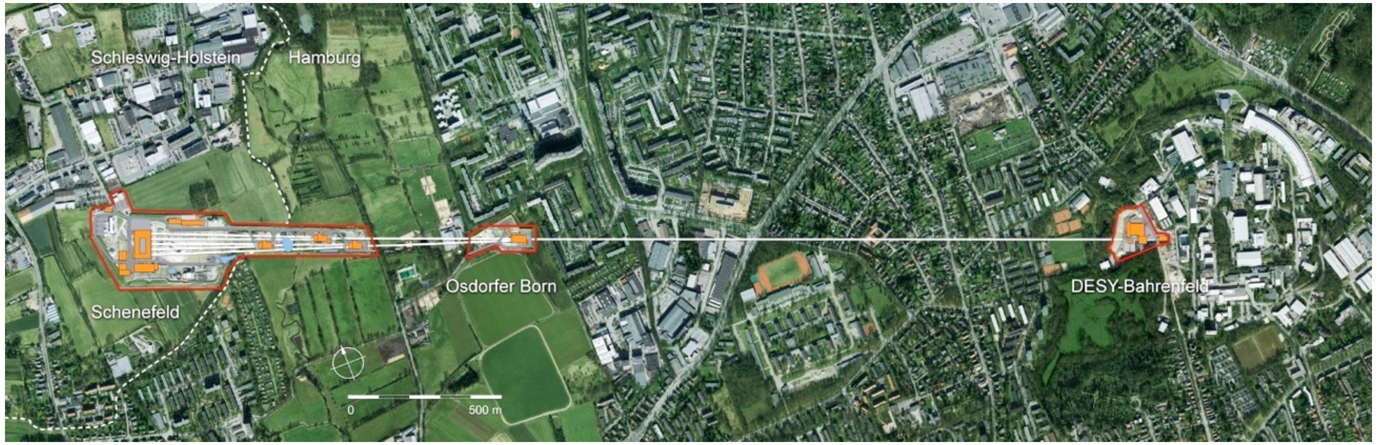
August 22, 2023

Outline

- Introduction to the European XFEL
- SFX at the European XFEL
- The data challenge: storage space and reuse options
- The way forward

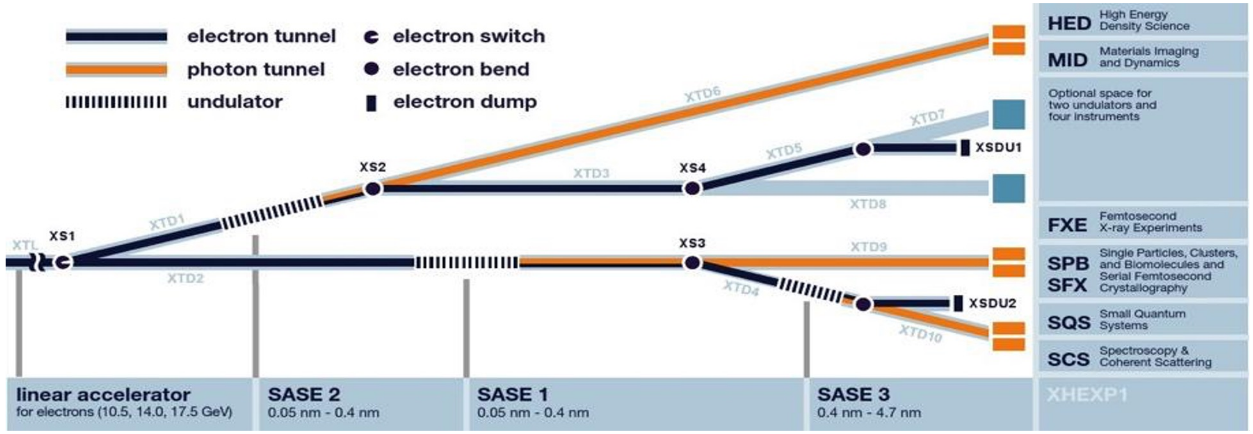
European XFEL at a glance

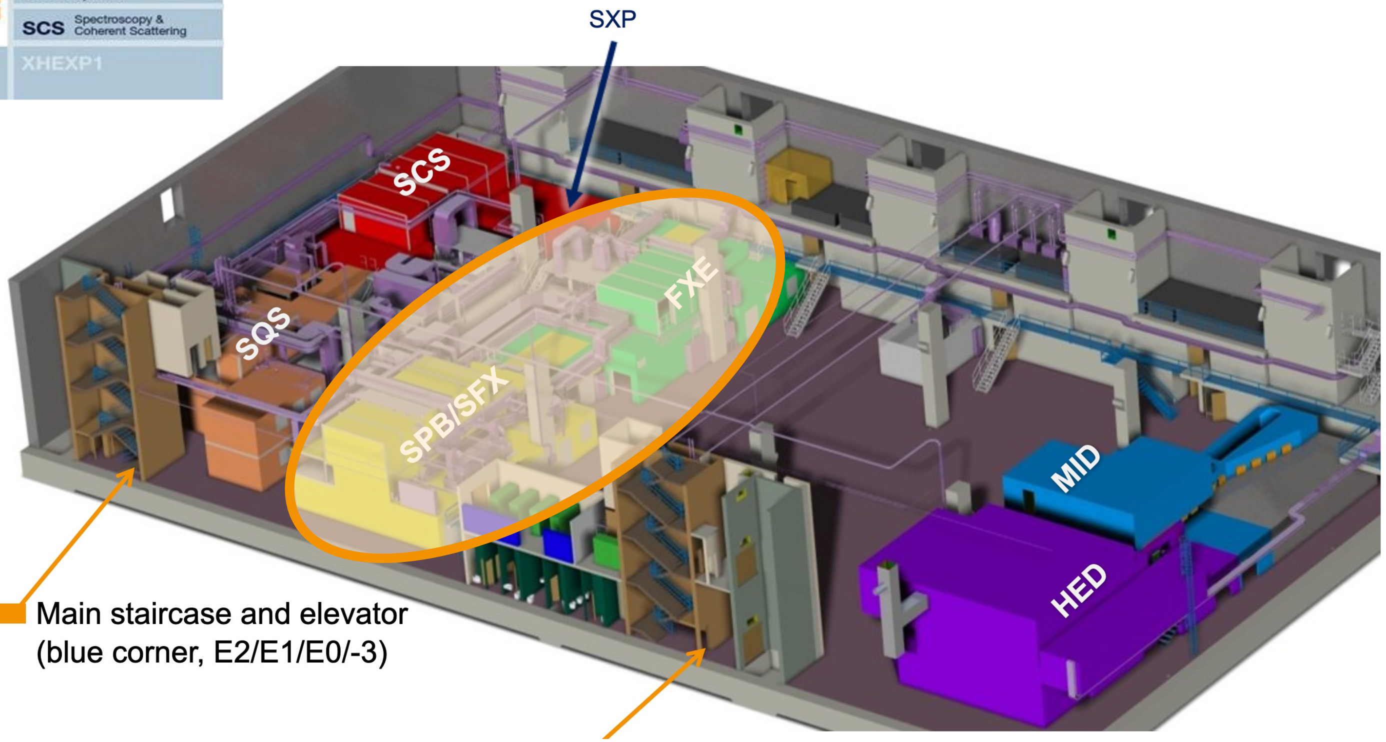
- Non-profit company, eleven shareholder countries
- Photon science user facility (plus own science), operation since September 2017
- currently > 500 employees



- linear electron accelerator, 3.4 km tunnel
- Seven scientific instruments

Beamlines and instruments

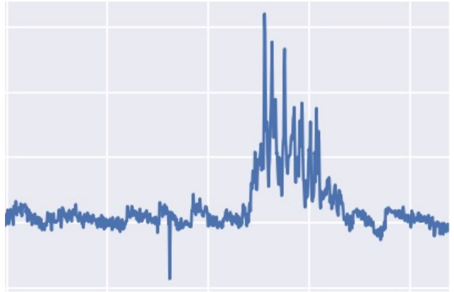

electron tunnel
photon tunnel
undulator
electron switch
electron bend
electron dump
XTL
XS1
XTD1
XTD2
XS2
XTD3
XTD6
XS4
XTD5
XTD7
XSDU1
XTD8
XS3
XTD9
XTD4
XSDU2
XTD10
HED High Energy Density Science
MID Materials Imaging and Dynamics
Optional space for two undulators and four instruments
FXE Femtosecond X-ray Experiments
SPB SFX Single Particles, Clusters, and Biomolecules and Serial Femtosecond Crystallography
SQS Small Quantum Systems
SCS Spectroscopy & Coherent Scattering
linear accelerator for electrons (10.5, 14.0, 17.5 GeV)
SASE 2 0.05 nm - 0.4 nm
SASE 1 0.05 nm - 0.4 nm
SASE 3 0.4 nm - 4.7 nm
XHEXP1

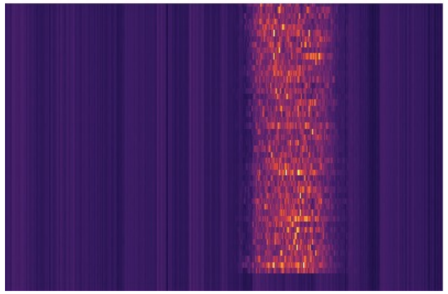


Main staircase and elevator (blue corner, E2/E1/E0/-3)

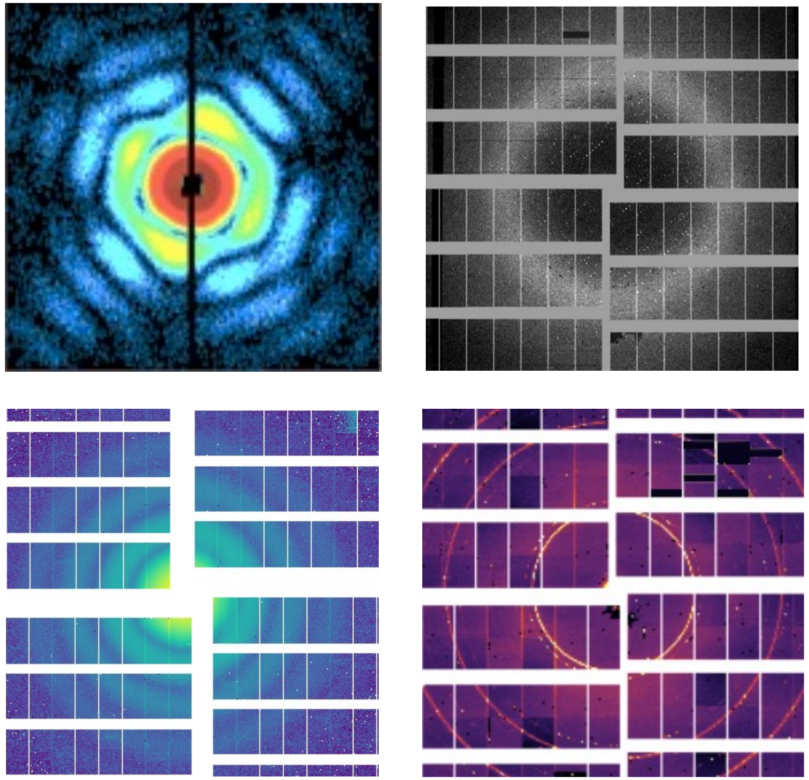
Major types of data

- Diffraction / scattering data: pixel / area detectors
  - integrating, mainly custom-built, multi-gain, MHz (burst mode)
- Spectroscopic data: 1D detectors, partly pulse-resolved (e. g. Gotthard)





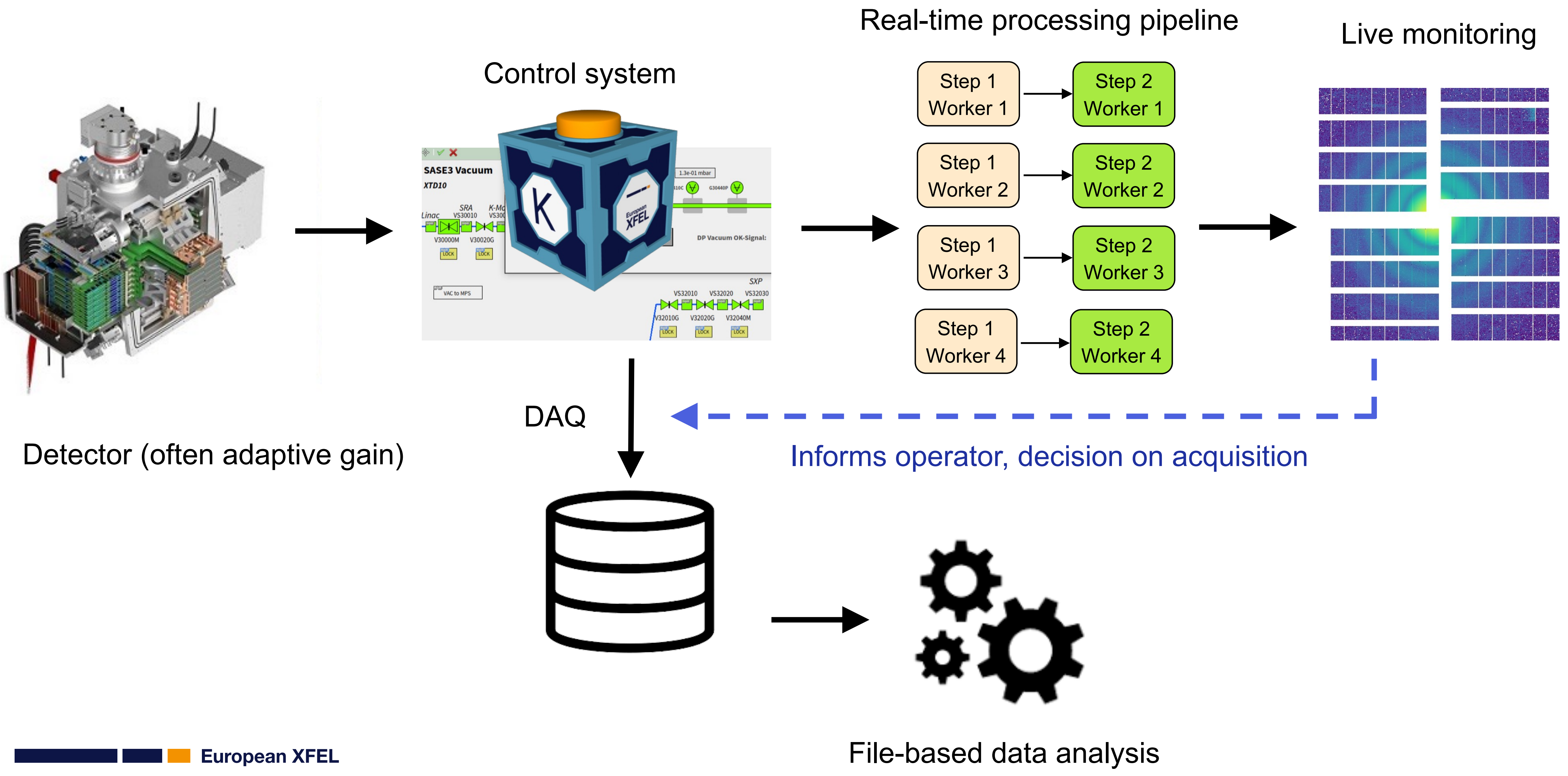
- Digitizers, diagnostics devices X-ray-gas monitors etc., control data (motors, valves etc.)...



[1]

[1] taken from Kirkwood et al. (2022) Nat. Sci. Data 9

Flow of experiment data



Control system

Real-time processing pipeline

Live monitoring

Step 1 Worker 1 → Step 2 Worker 1

Step 1 Worker 2 → Step 2 Worker 2

Step 1 Worker 3 → Step 2 Worker 3

Step 1 Worker 4 → Step 2 Worker 4

DAQ

Detector (often adaptive gain)

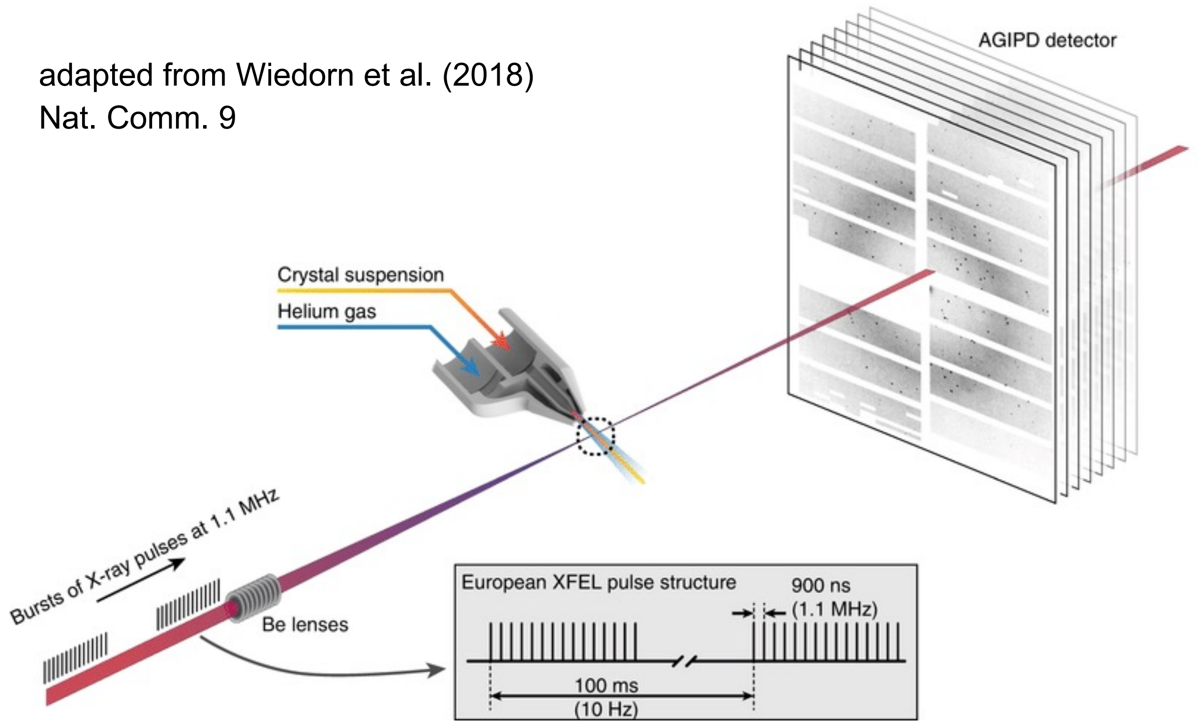
Informs operator, decision on acquisition

File-based data analysis

SFX at the European XFEL

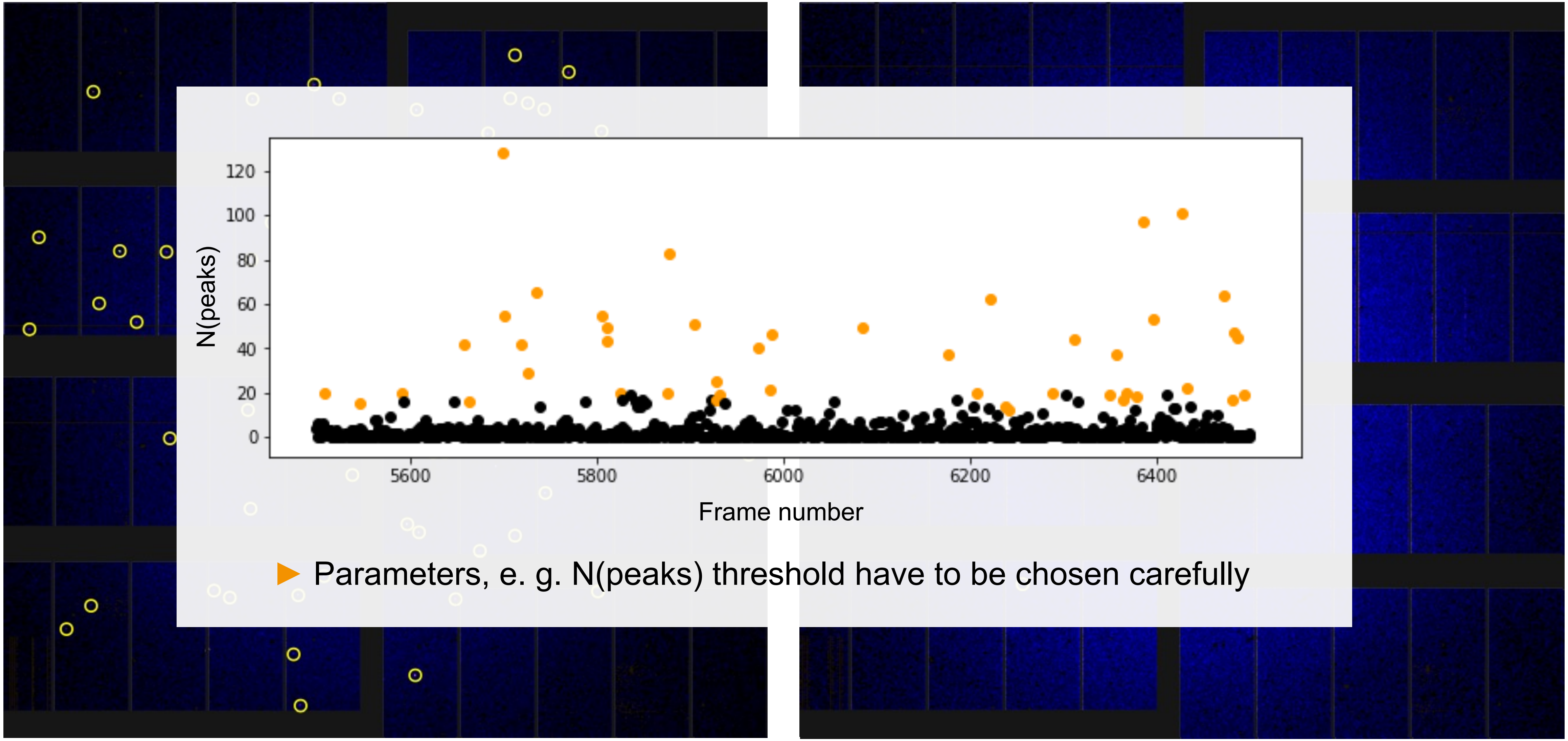
The typical SFX setup at EuXFEL (SPB/SFX)

adapted from Wiedorn et al. (2018)
Nat. Comm. 9



- Diffraction before destruction
- Each image stems from a differently oriented crystal, indexing cannot make use of multi-frame information
- Requirement of high crystal isomorphism, each image must represent (closely) the same crystal “template”
- Still images, no oscillation range, integration must use a 3D model for 2D pixel data
- Many empty frames due to missing shots

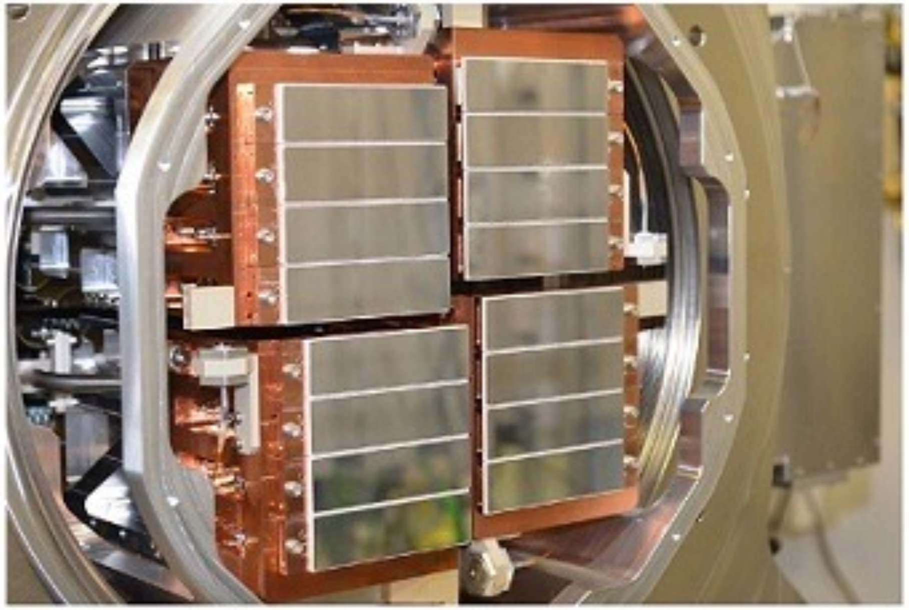
Crystal hits and misses

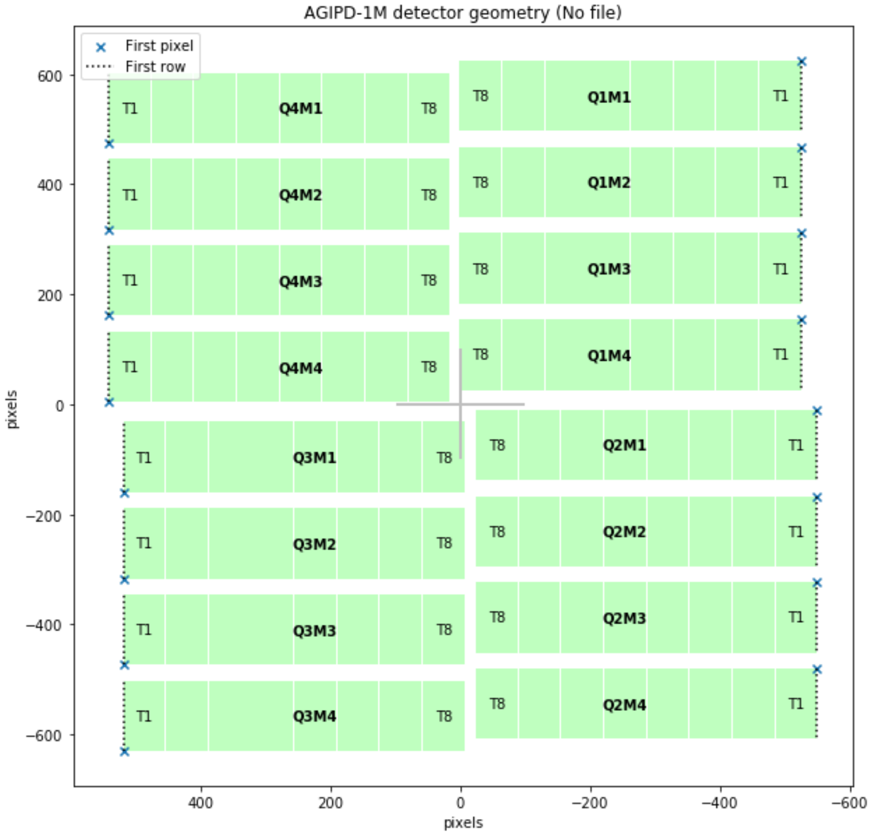


- Parameters, e. g. N(peaks) threshold have to be chosen carefully

SPB/SFX, AGIPD-1M

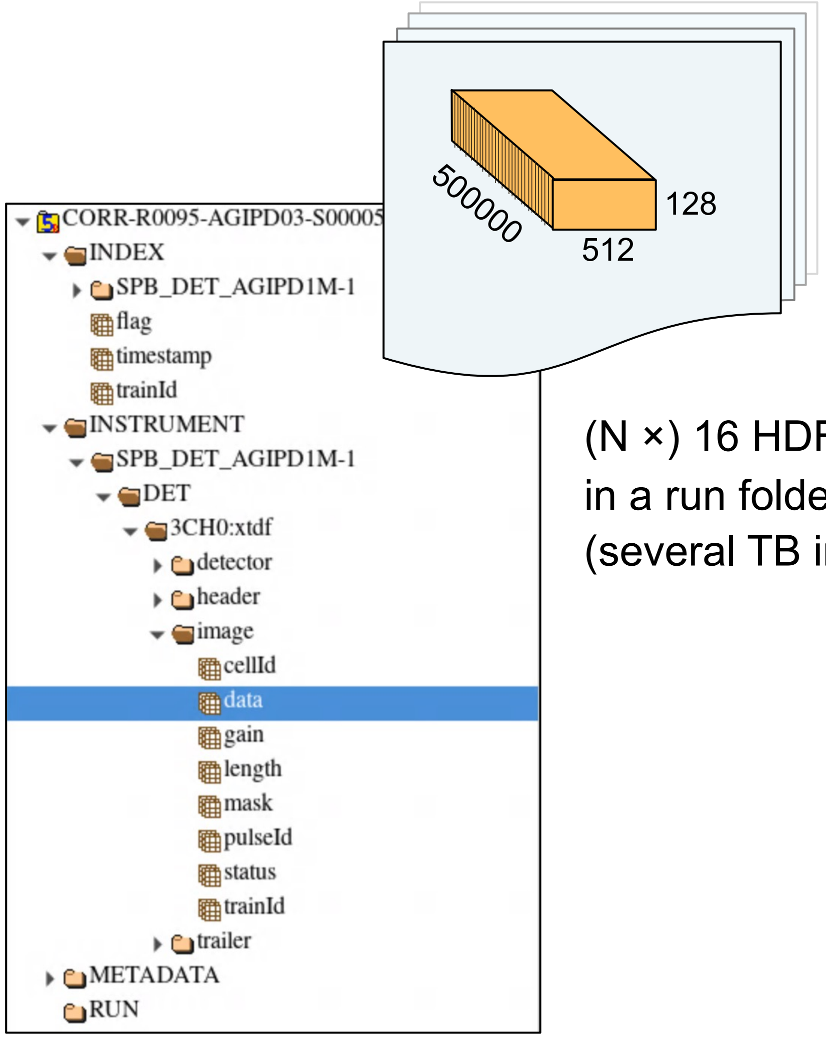
Detectors: multi-module topology





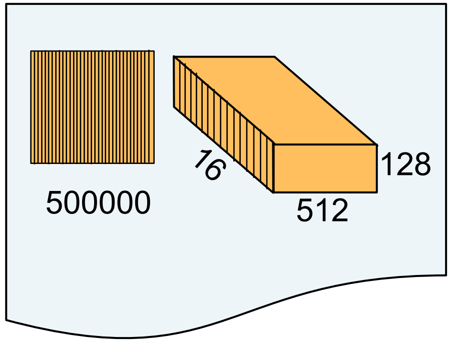
- AGIPD-1M detector, 16 modules, separate read-out
- four quadrants of four modules, motor-moveable

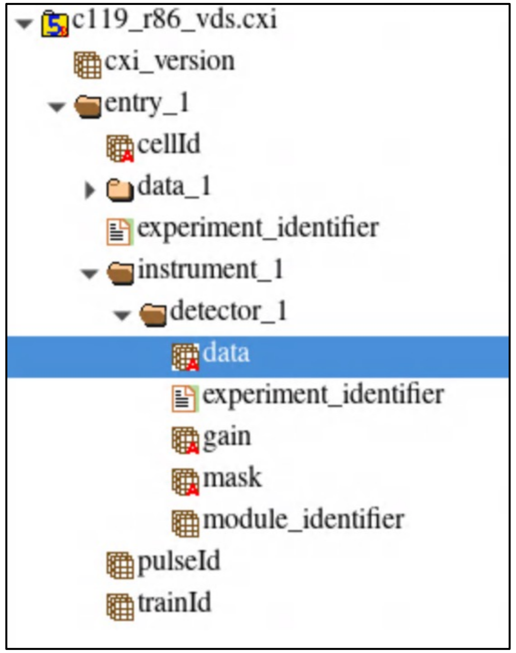
Data format / shape



- CORR-R0095-AGIPD03-S00005
  - INDEX
    - SPB_DET_AGIPD1M-1
    - flag
    - timestamp
    - trainId
  - INSTRUMENT
    - SPB_DET_AGIPD1M-1
      - DET
        - 3CH0:xtdf
          - detector
          - header
          - image
            - cellId
            - data
            - gain
            - length
            - mask
            - pulseId
            - status
            - trainId
          - trailer
  - METADATA
  - RUN

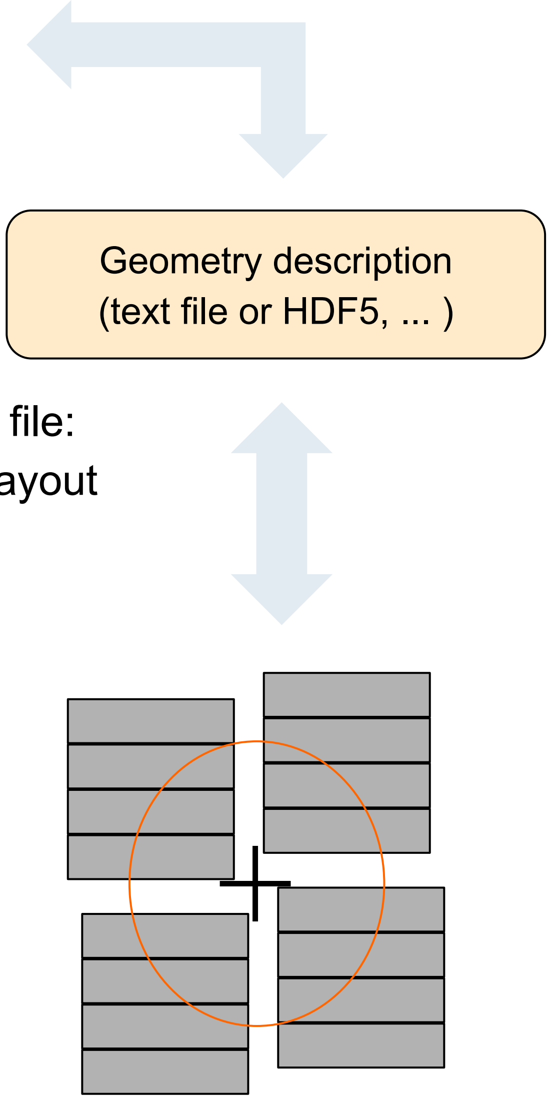
(N ×) 16 HDF5 files
in a run folder
(several TB in total)





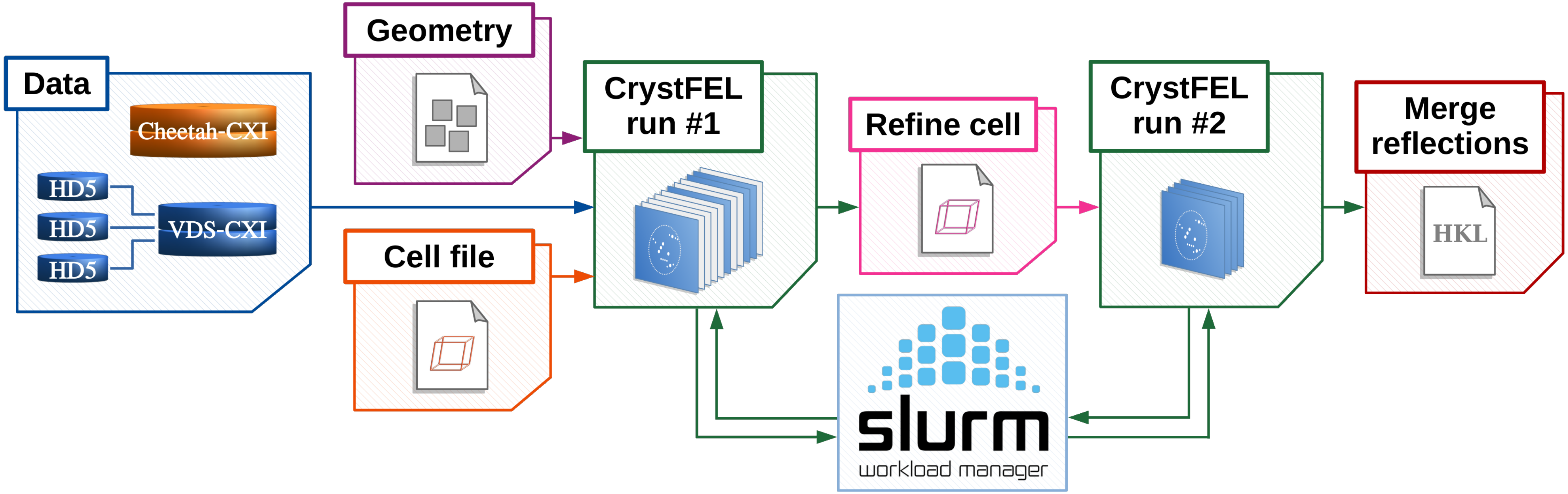
- c119_r86_vds.cxi
  - cxi_version
  - entry_1
    - cellId
    - data_1
    - experiment_identifier
    - instrument_1
      - detector_1
        - data
        - experiment_identifier
        - gain
        - mask
        - module_identifier
    - pulseId
    - trainId

single HDF5 file:
virtual data layout
(~ 50 MB)



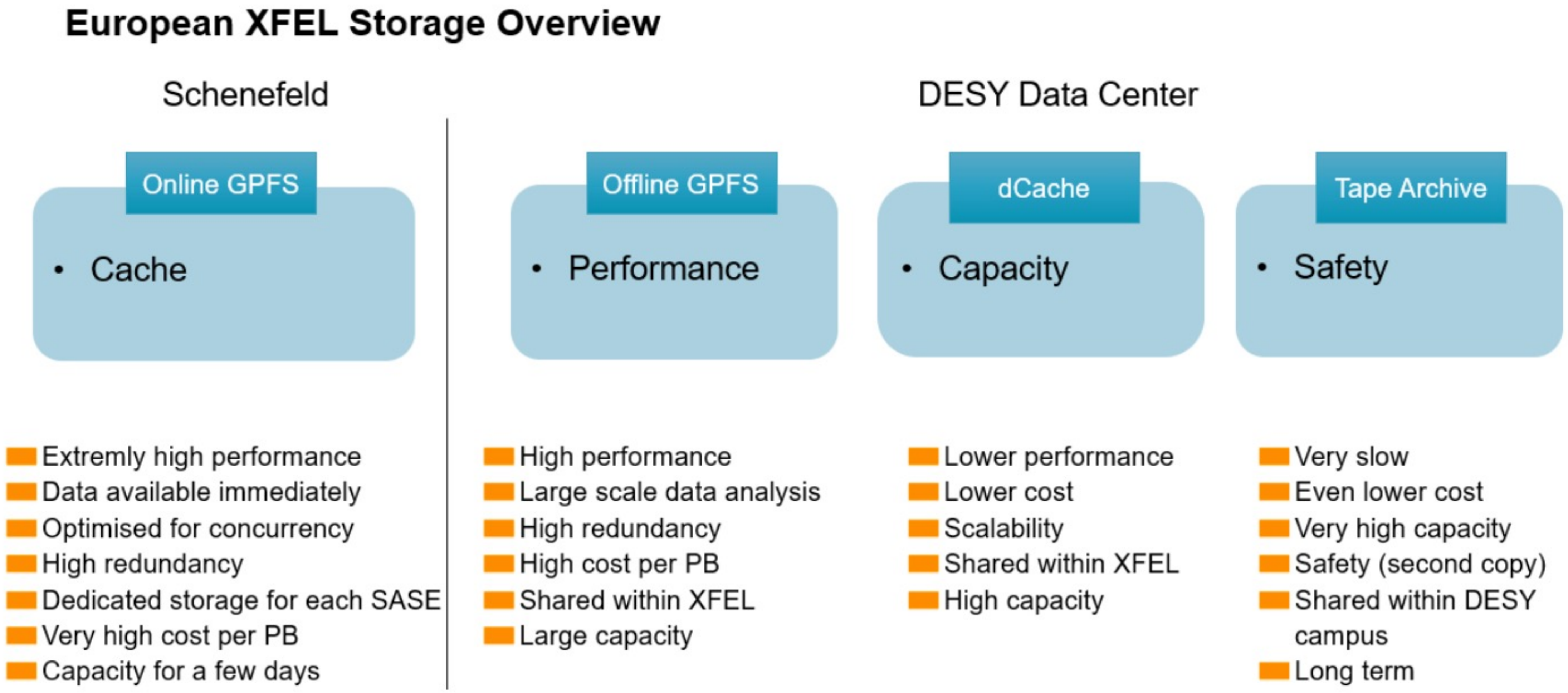
Geometry description
(text file or HDF5, ...)

Extra-Xwiz is a pipeline for data processing with CrystFEL



The data challenge: storage space and re-use options

File systems for data storage



European XFEL Storage Overview

Schenefeld

Online GPFS

- Cache

- Extrmly high performance
- Data available immediately
- Optimised for concurrency
- High redundancy
- Dedicated storage for each SASE
- Very high cost per PB
- Capacity for a few days

DESY Data Center

Offline GPFS

- Performance

- High performance
- Large scale data analysis
- High redundancy
- High cost per PB
- Shared within XFEL
- Large capacity

dCache

- Capacity

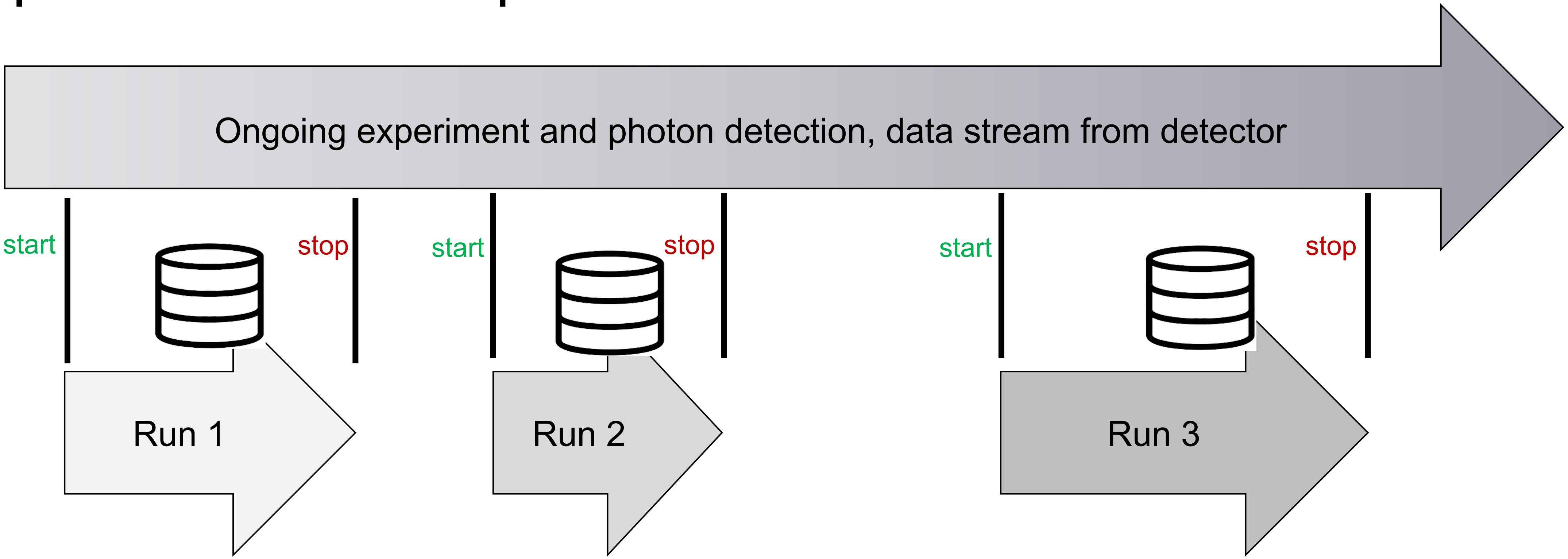
- Lower performance
- Lower cost
- Scalability
- Shared within XFEL
- High capacity

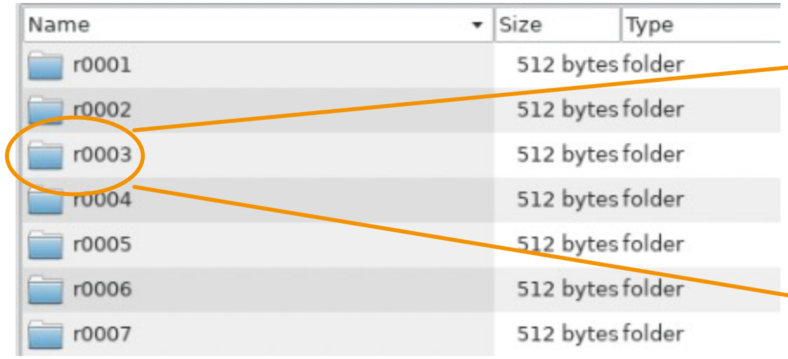
Tape Archive

- Safety

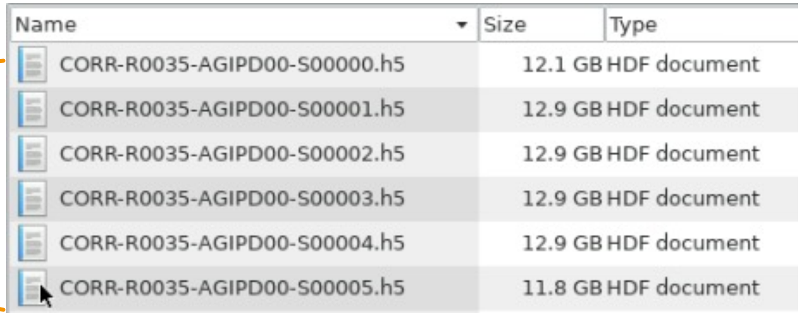
- Very slow
- Even lower cost
- Very high capacity
- Safety (second copy)
- Shared within DESY campus
- Long term

Experiment data acquisition to runs


Ongoing experiment and photon detection, data stream from detector
start
stop
Run 1
start
stop
Run 2
start
stop
Run 3

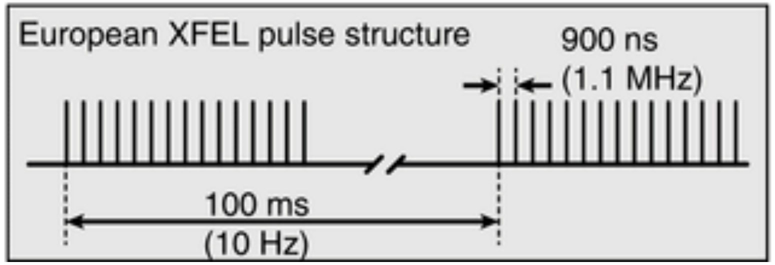


Name	Size	Type
r0001	512 bytes	folder
r0002	512 bytes	folder
r0003	512 bytes	folder
r0004	512 bytes	folder
r0005	512 bytes	folder
r0006	512 bytes	folder
r0007	512 bytes	folder

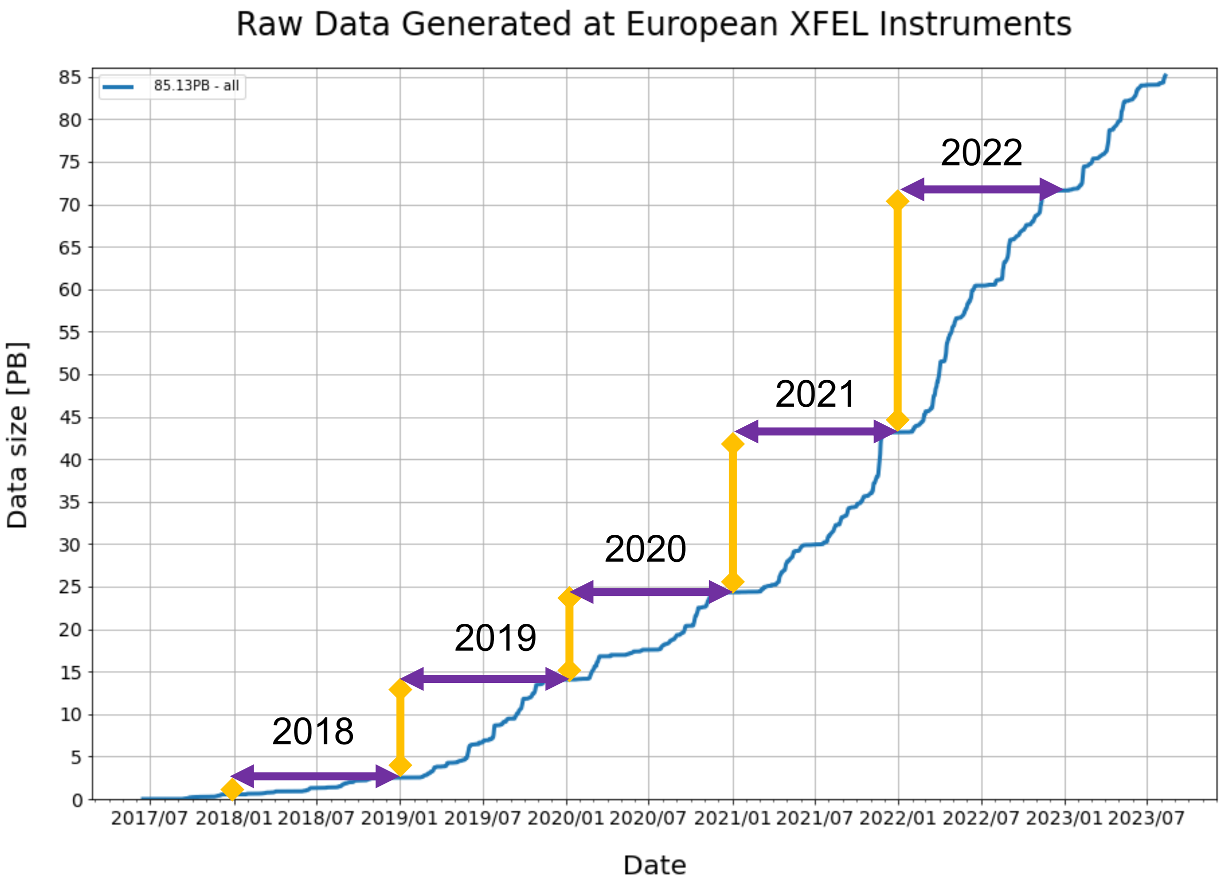


Name	Size	Type
CORR-R0035-AGIPD00-S00000.h5	12.1 GB	HDF document
CORR-R0035-AGIPD00-S00001.h5	12.9 GB	HDF document
CORR-R0035-AGIPD00-S00002.h5	12.9 GB	HDF document
CORR-R0035-AGIPD00-S00003.h5	12.9 GB	HDF document
CORR-R0035-AGIPD00-S00004.h5	12.9 GB	HDF document
CORR-R0035-AGIPD00-S00005.h5	11.8 GB	HDF document

Volume of stored data



- accelerator can produce up to 27000 pulses per second (4.4 MHz max intra-train)
- detectors sync to pulse-train structure, typically 3500 to 8000 frames / second
- maximum of 52 TB/h (for the most frequent MHz detector), up to 4 PB raw data per beam-time, assuming highest efficiency

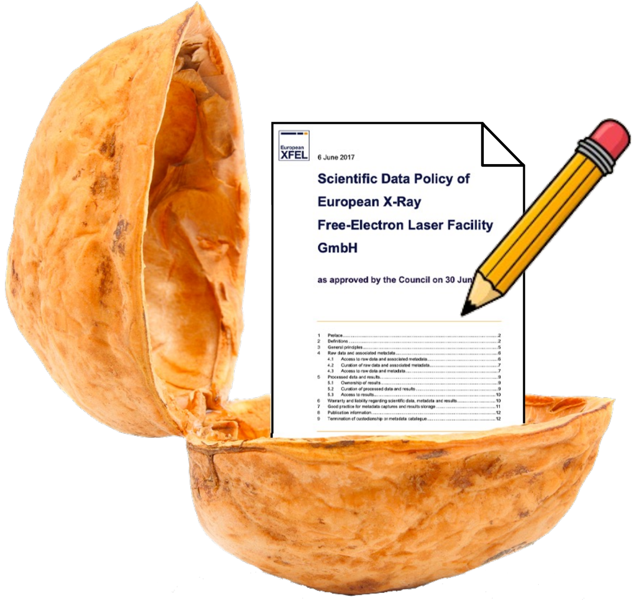


Krzysztof Wrona & Janusz Malka

- Experimental efficiency in terms of data taking time fraction has increased within the last year

The EuXFEL scientific data policy in a nutshell

- Follows PaN Data Europe WG recommendations (2011)
- Users accept it to get beam-time awarded
- Raw data are embargoed for 3 years
  - then become automatically open (not stated what this exactly means)
- Access to results-data is restricted
- Derived data are not retained long-term
  - best-effort curation by EuXFEL, but not including e.g. SW for reproducibility
- Metadata: "good practice is encouraged" (no mention of concrete arrangements)



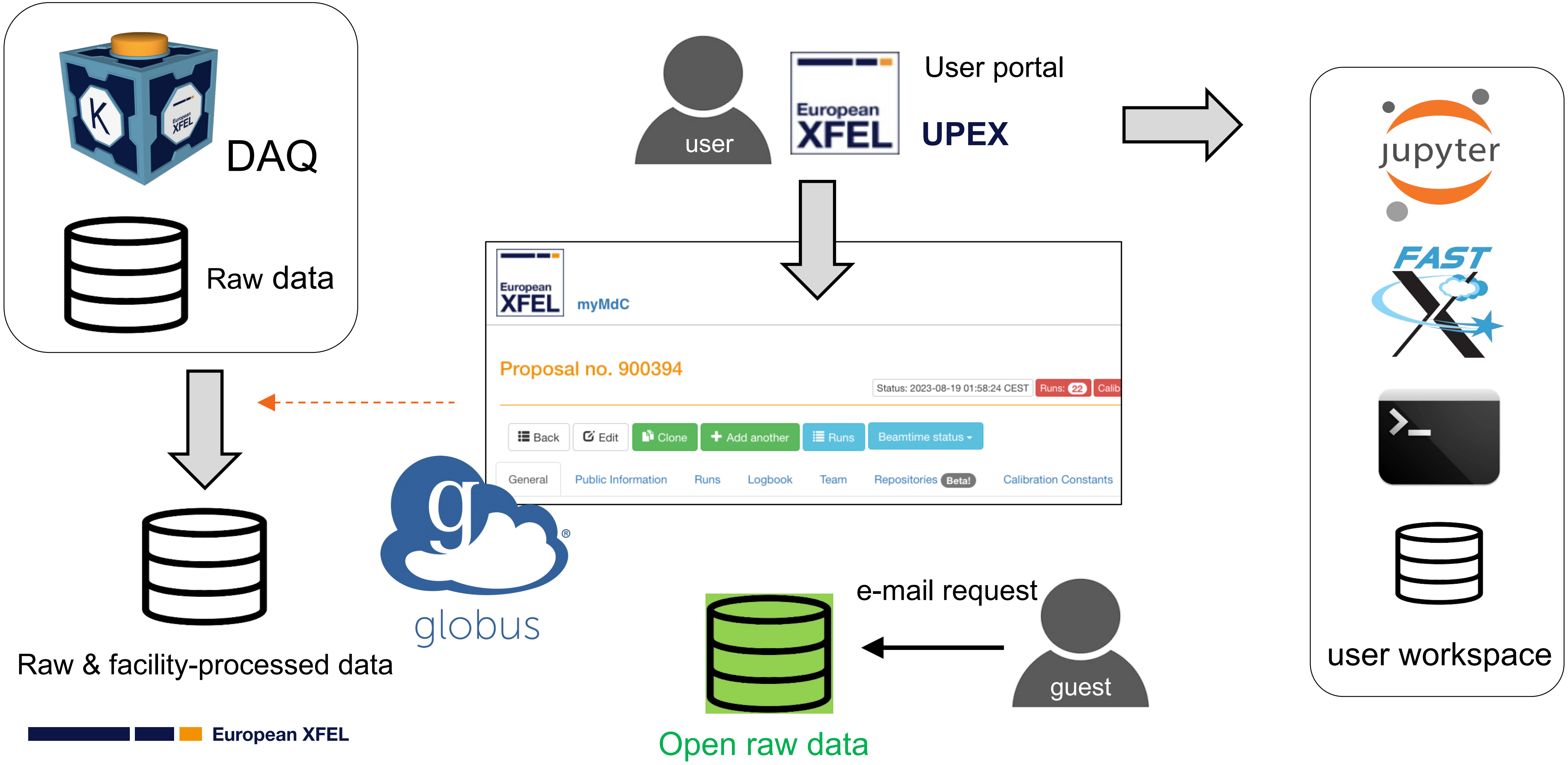
European XFEL

6 June 2017

Scientific Data Policy of European X-Ray Free-Electron Laser Facility GmbH

as approved by the Council on 30 Jun

Access of EuXFEL data via myMDC



DAQ

Raw data

user

European XFEL

User portal

UPEX

European XFEL myMdC

Proposal no. 900394

Status: 2023-08-19 01:58:24 CEST | Runs: 22 | Calib

Back | Edit | Clone | Add another | Runs | Beamtime status

General | Public Information | Runs | Logbook | Team | Repositories Beta! | Calibration Constants

globus

Raw & facility-processed data

e-mail request

guest

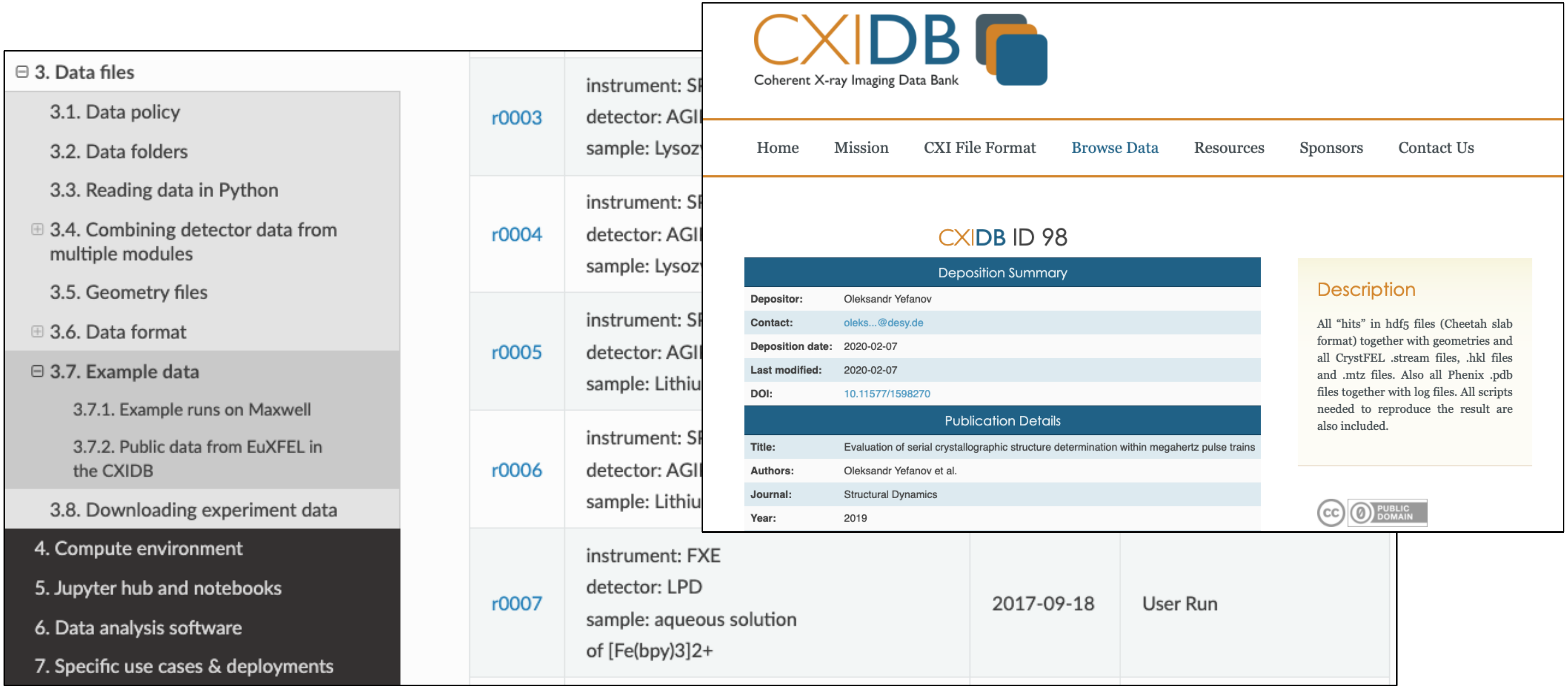
Open raw data

jupyter

FAST X

user workspace

Open SFX data from EuXFEL



⊟ 3. Data files

- 3.1. Data policy
- 3.2. Data folders
- 3.3. Reading data in Python
- ⊞ 3.4. Combining detector data from multiple modules
- 3.5. Geometry files
- ⊞ 3.6. Data format
- ⊟ 3.7. Example data
  - 3.7.1. Example runs on Maxwell
  - 3.7.2. Public data from EuXFEL in the CXIDB
- 3.8. Downloading experiment data

4. Compute environment

5. Jupyter hub and notebooks

6. Data analysis software

7. Specific use cases & deployments

r0003	instrument: SP detector: AGI sample: Lysoz		
r0004	instrument: SP detector: AGI sample: Lysoz		
r0005	instrument: SP detector: AGI sample: Lithiu		
r0006	instrument: SP detector: AGI sample: Lithiu		
r0007	instrument: FXE detector: LPD sample: aqueous solution of [Fe(bpy)3]2+	2017-09-18	User Run

CXIDB
Coherent X-ray Imaging Data Bank

CXIDB ID 98

Deposition Summary

Depositor:	Oleksandr Yefanov
Contact:	oleks...@desy.de
Deposition date:	2020-02-07
Last modified:	2020-02-07
DOI:	10.11577/1598270

Publication Details

Title:	Evaluation of serial crystallographic structure determination within megahertz pulse trains
Authors:	Oleksandr Yefanov et al.
Journal:	Structural Dynamics
Year:	2019

Description

All "hits" in hdf5 files (Cheetah slab format) together with geometries and all CrystFEL .stream files, .hkl files and .mtz files. Also all Phenix .pdb files together with log files. All scripts needed to reproduce the result are also included.

CC 0 PUBLIC DOMAIN

The PaNOSC project

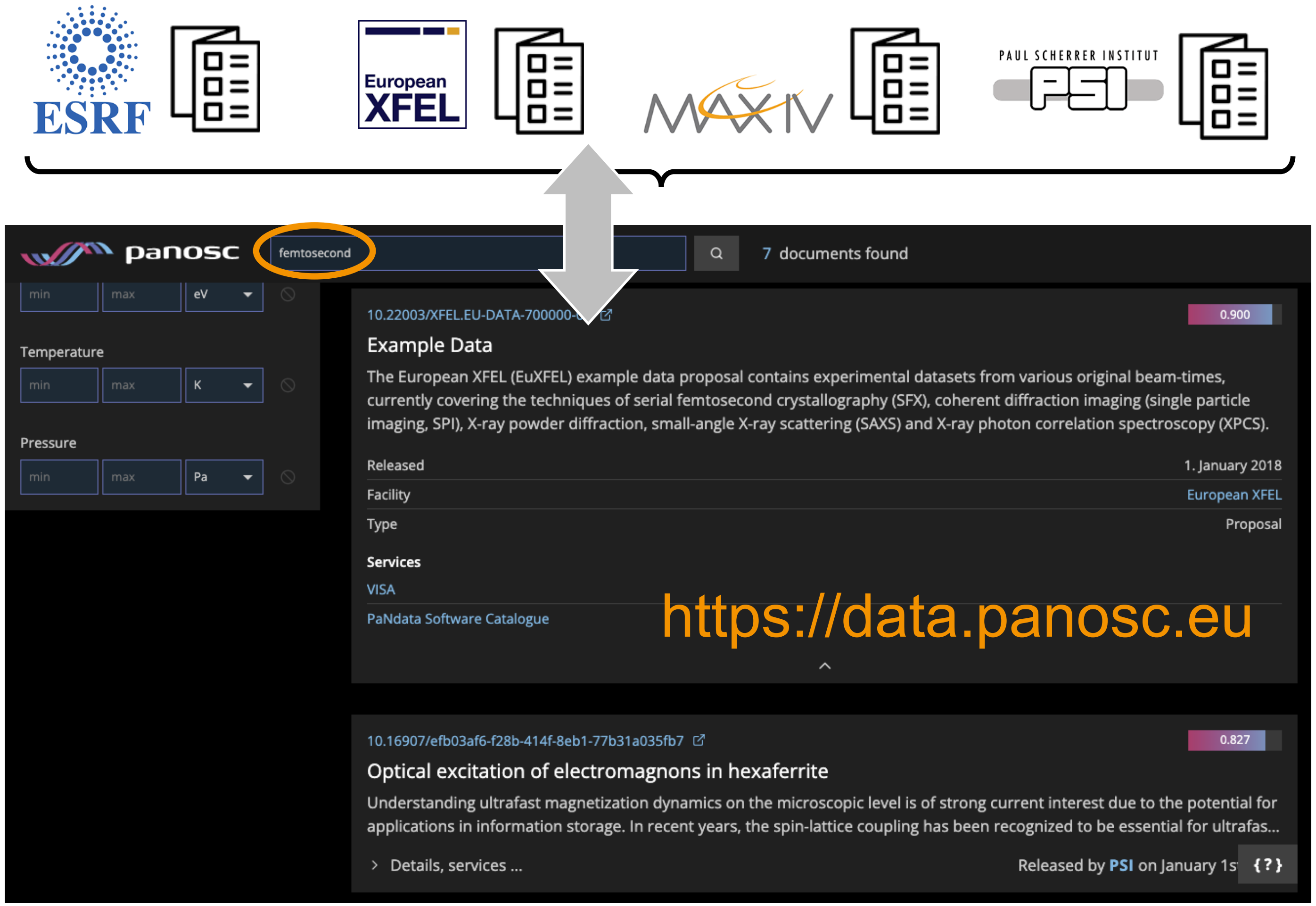
- EuXFEL was one of six contributing PaN facilities, 2018-2022
- Outcomes include:
  - FAIR recommendations for PaN data
  - Data analysis software and remote data analysis services
  - Simulation software
  - Solutions for unified authentication and other federated services
  - Training resources (learning platform, summer schools)

What is the difference between “FAIR data” and “Open data” if there is one?

- Open data and FAIR data are two related but different things
- Openness lies in the A of FAIR, access levels (authentication, authorization) need to be adjusted case by case

Finding open EuXFEL data: the PaN search portal

Example data from real experiments (XMPL)



femtosecond

7 documents found

min max eV

Temperature

min max K

Pressure

min max Pa

10.22003/XFEL.EU-DATA-700000- 0.900

Example Data

The European XFEL (EuXFEL) example data proposal contains experimental datasets from various original beam-times, currently covering the techniques of serial femtosecond crystallography (SFX), coherent diffraction imaging (single particle imaging, SPI), X-ray powder diffraction, small-angle X-ray scattering (SAXS) and X-ray photon correlation spectroscopy (XPCS).

Released	1. January 2018
Facility	European XFEL
Type	Proposal

Services

VISA

PaNdata Software Catalogue

https://data.panosc.eu

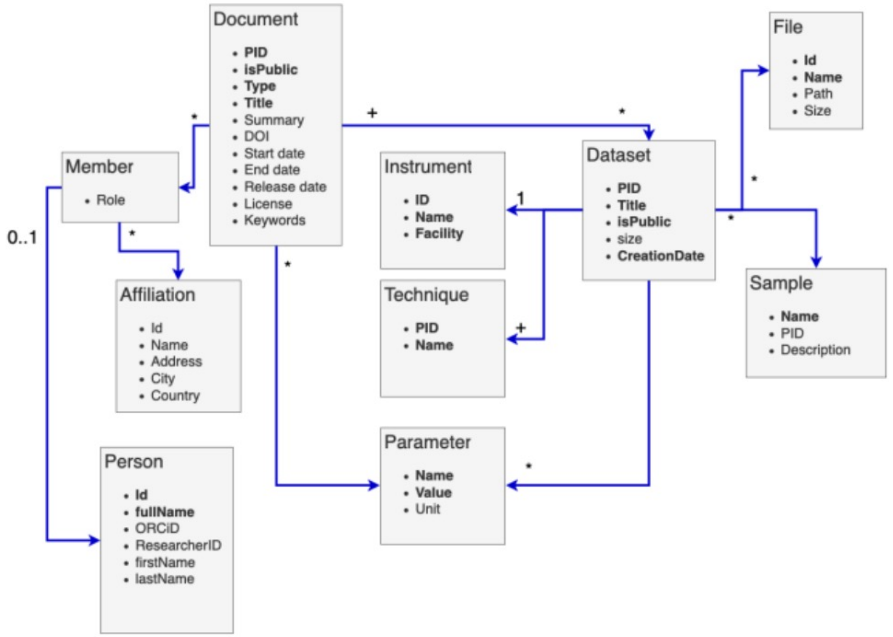
10.16907/efb03af6-f28b-414f-8eb1-77b31a035fb7 0.827

Optical excitation of electromagnons in hexaferrite

Understanding ultrafast magnetization dynamics on the microscopic level is of strong current interest due to the potential for applications in information storage. In recent years, the spin-lattice coupling has been recognized to be essential for ultrafas...

Details, services ...

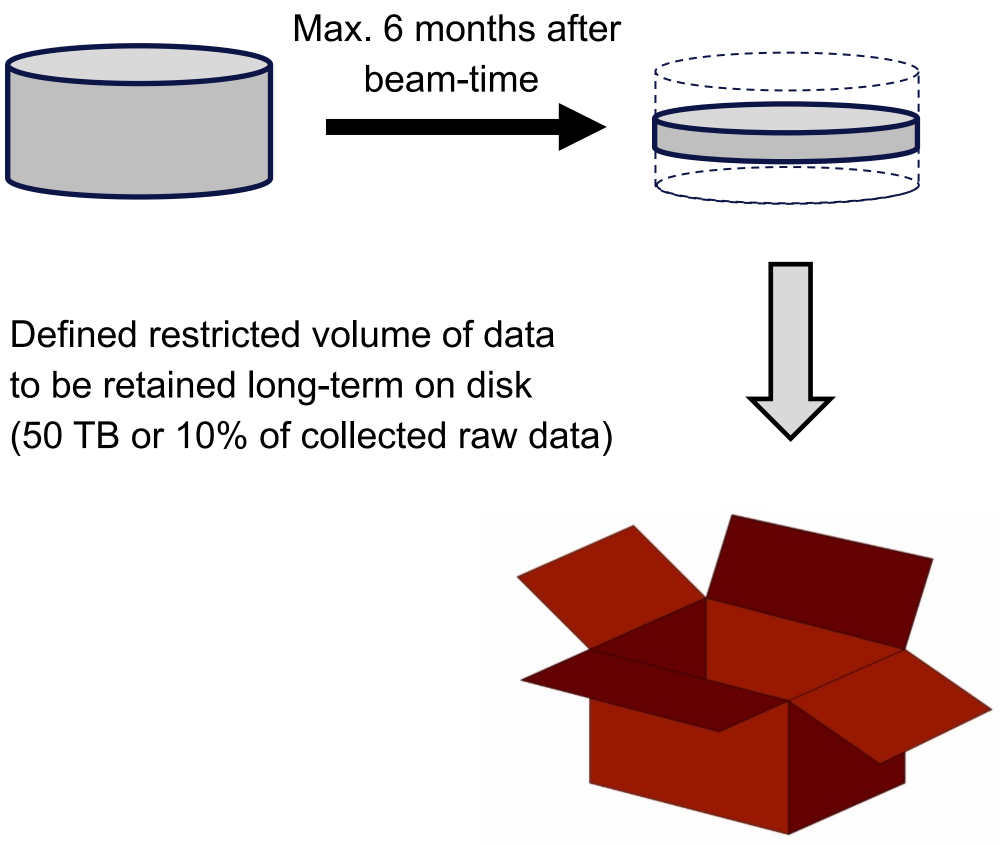
Released by PSI on January 1s {?}



- Metadata model of common items for search and filter terms
  - Agreed-on subset, intersection of different catalogue systems
  - PaNET ontology for experimental techniques

The way forward

Data reduction - the aim



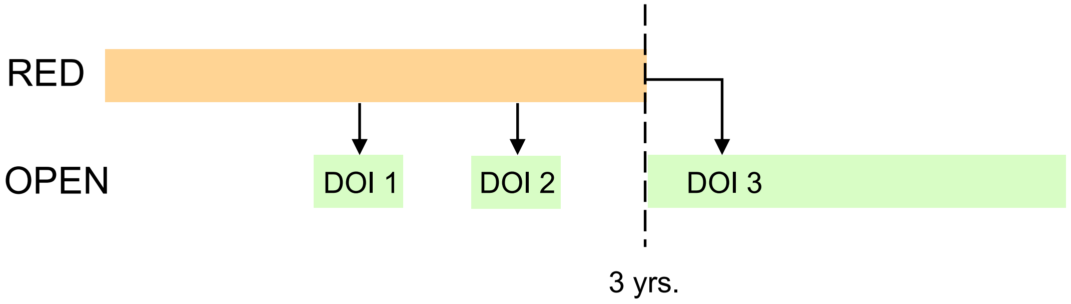
Max. 6 months after beam-time

Defined restricted volume of data
to be retained long-term on disk
(50 TB or 10% of collected raw data)

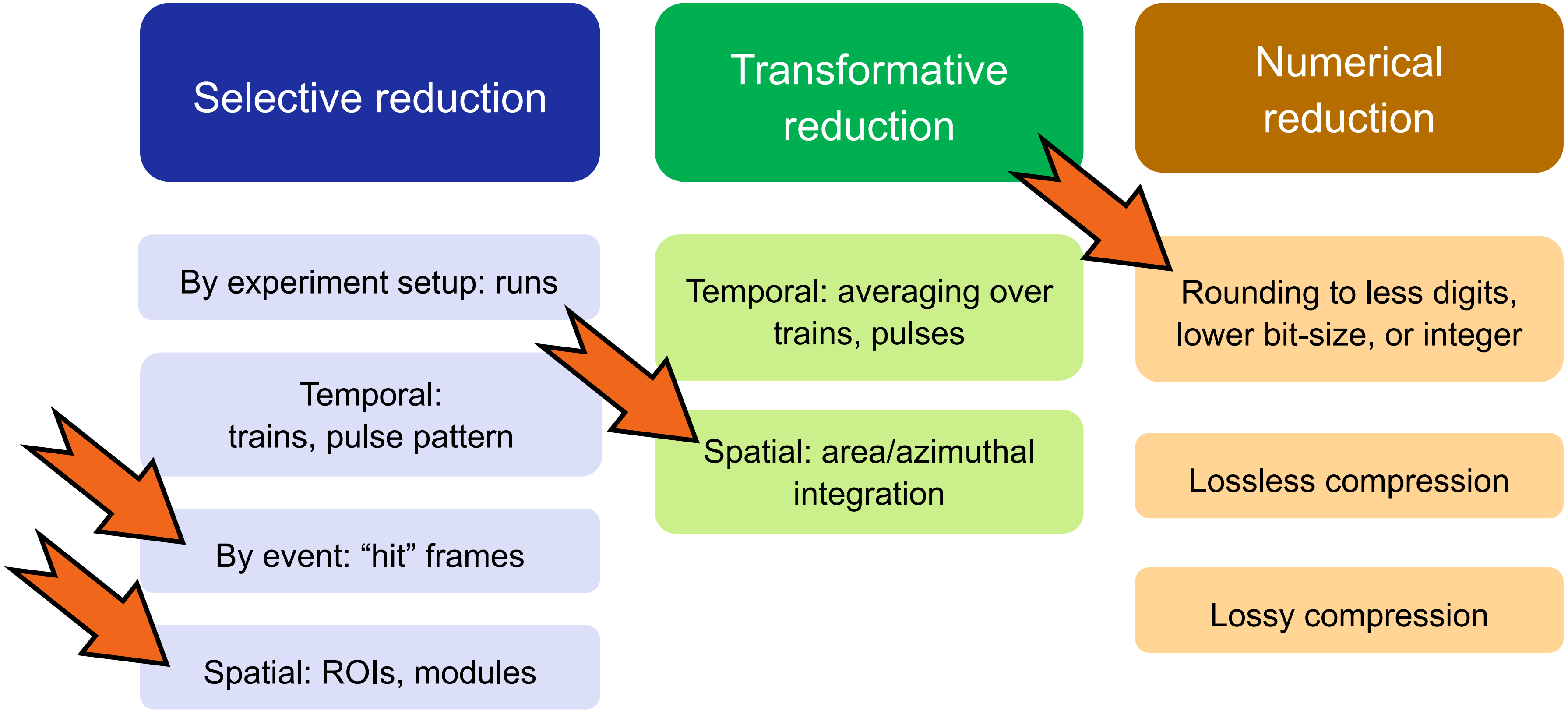
Optional content of the RED data volume

- Selected runs of raw data
- All runs of raw data with event-selected detector frames
- Only processed data, likely selected and/or reduced, including corrected data in European XFEL format
- A mixture of selected raw data and processed data

RED data becomes OPEN data automatically after end of the embargo period, allowing for earlier OPEN data subsets upon publication



Data reduction - the methods



Selective reduction

- By experiment setup: runs
- Temporal: trains, pulse pattern
- By event: “hit” frames
- Spatial: ROIs, modules

Transformative reduction

- Temporal: averaging over trains, pulses
- Spatial: area/azimuthal integration

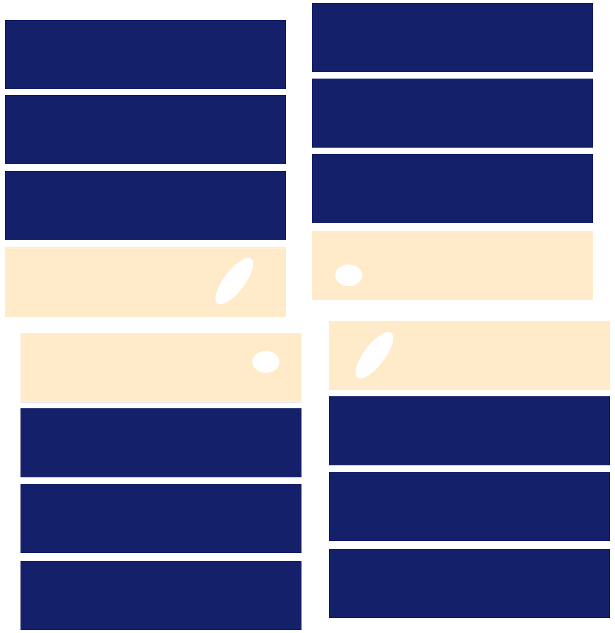
Numerical reduction

- Rounding to less digits, lower bit-size, or integer
- Lossless compression
- Lossy compression

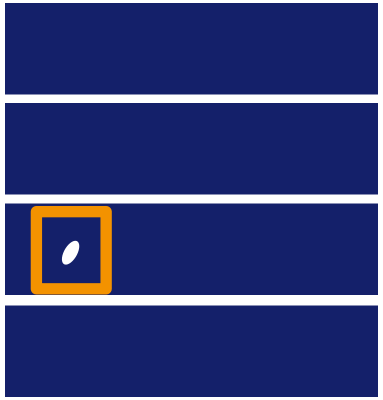
- Most of these methods are performed in users’ data analysis “anyway”
- In the context of the RED process, these methods will be implemented to facility procedures and deployed as largely automated services

Data reduction – conceptual examples

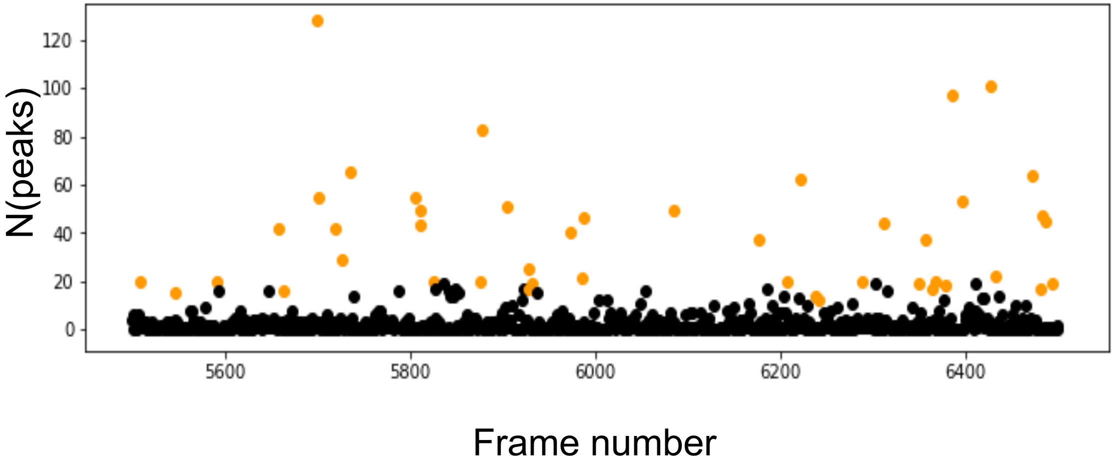
I



II



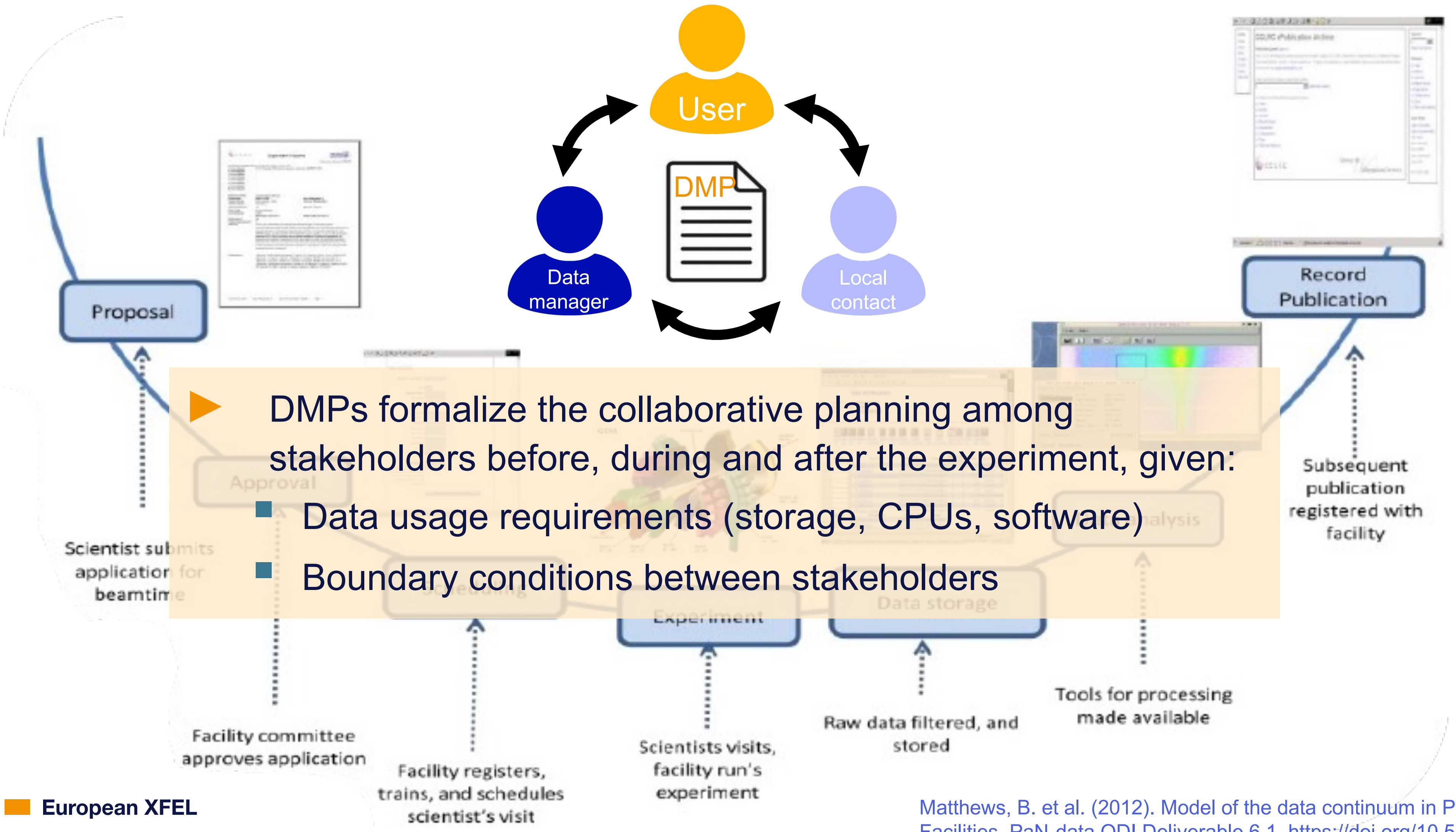
III



Spatial selection (modules, ROIs)

Event selection

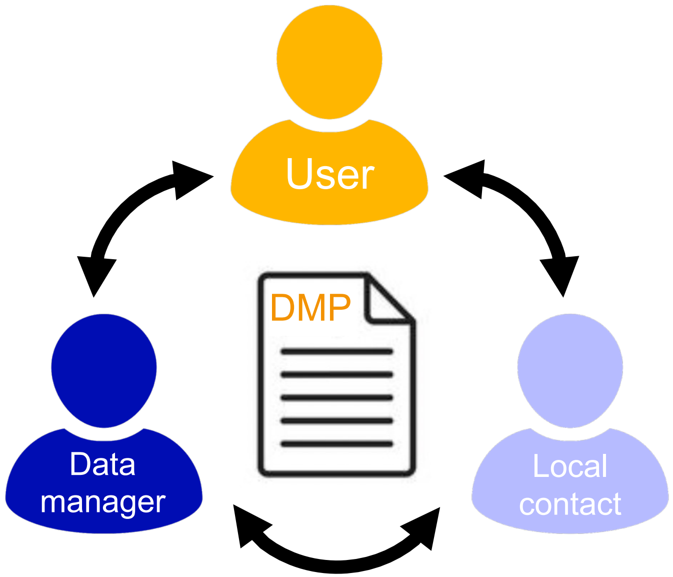
Data lifecycle and data management plans


User
DMP
Data manager
Local contact
Proposal
Approval
Scheduling
Experiment
Data storage
Analysis
Record Publication
Scientist submits application for beamtime
Facility committee approves application
Facility registers, trains, and schedules scientist's visit
Scientists visits, facility run's experiment
Raw data filtered, and stored
Tools for processing made available
Subsequent publication registered with facility

- DMPs formalize the collaborative planning among stakeholders before, during and after the experiment, given:
  - Data usage requirements (storage, CPUs, software)
  - Boundary conditions between stakeholders

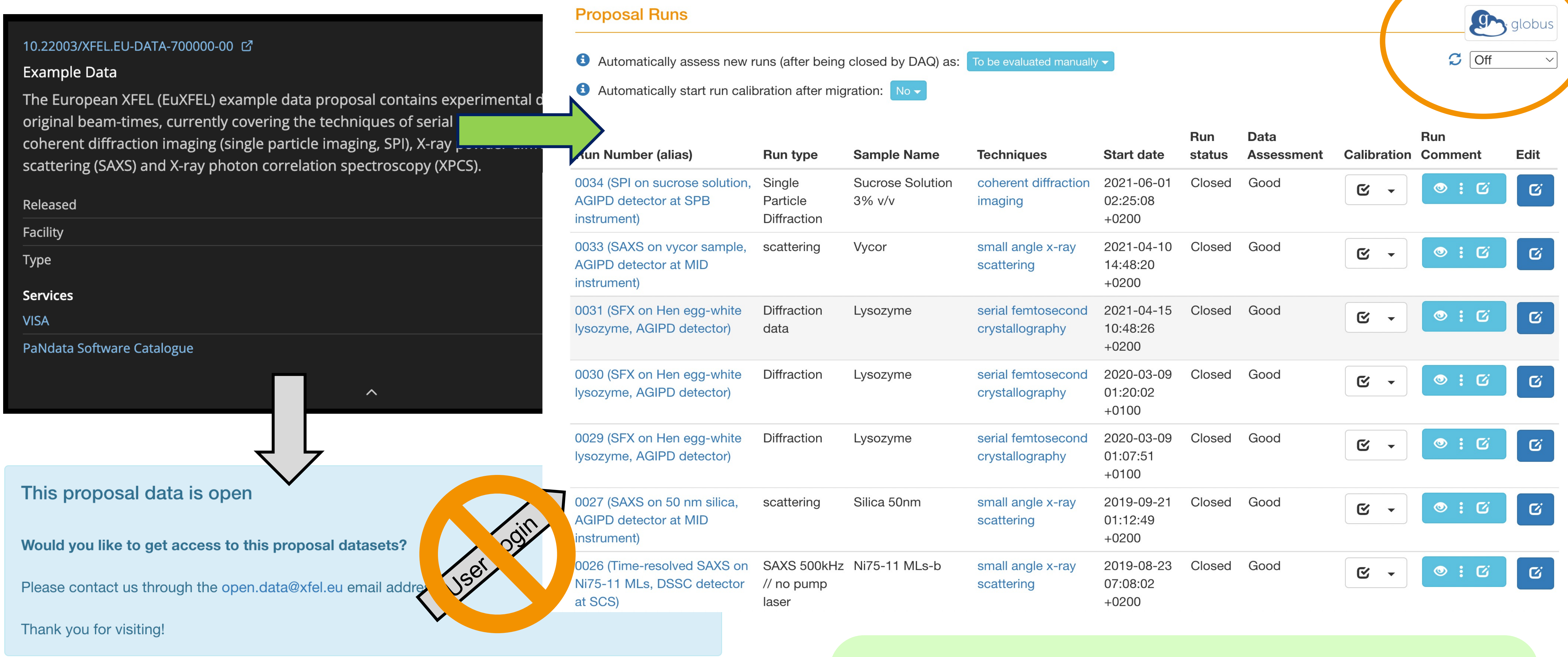
Matthews, B. et al. (2012). Model of the data continuum in Photon and Neutron Facilities. PaN-data ODI Deliverable 6.1. https://doi.org/10.5281/zenodo.3897910

Features of data management plans



- DMPs will be integrated to the existing facility workflow
- DMPs will be automatically pre-filled as much as possible with user office data and other proposal information
- DMPs are dynamic documents adapted at each stage from proposal acceptance to the open access phase
- DMPs will be editable by each of the partners, with automatic notification of changes

Open data access: integration to myMDC



10.22003/XFEL.EU-DATA-700000-00

Example Data

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scattering (SAXS) and X-ray photon correlation spectroscopy (XPCS).

Released

Facility

Type

Services

VISA

PaNdata Software Catalogue

This proposal data is open

Would you like to get access to this proposal datasets?

Please contact us through the open.data@xfel.eu email addre

Thank you for visiting!

Proposal Runs

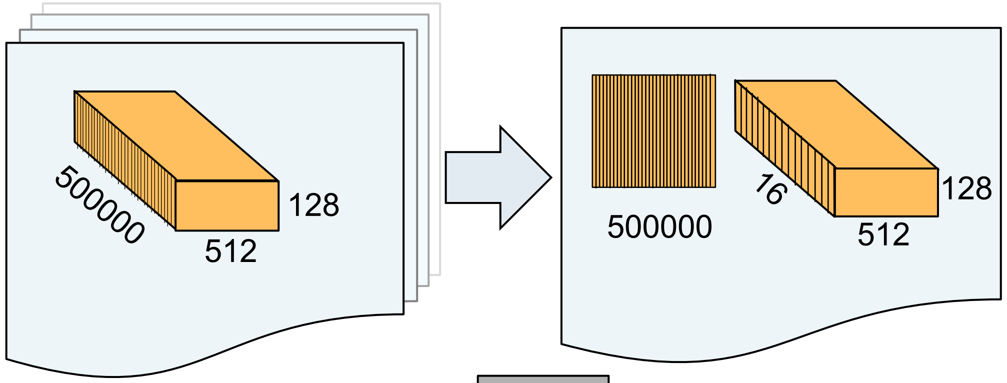
Automatically assess new runs (after being closed by DAQ) as: To be evaluated manually

Automatically start run calibration after migration: No

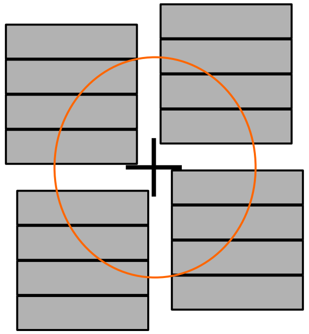
un Number (alias)	Run type	Sample Name	Techniques	Start date	Run status	Data Assessment	Calibration	Run Comment	Edit
0034 (SPI on sucrose solution, AGIPD detector at SPB instrument)	Single Particle Diffraction	Sucrose Solution 3% v/v	coherent diffraction imaging	2021-06-01 02:25:08 +0200	Closed	Good			
0033 (SAXS on vycor sample, AGIPD detector at MID instrument)	scattering	Vycor	small angle x-ray scattering	2021-04-10 14:48:20 +0200	Closed	Good			
0031 (SFX on Hen egg-white lysozyme, AGIPD detector)	Diffraction data	Lysozyme	serial femtosecond crystallography	2021-04-15 10:48:26 +0200	Closed	Good			
0030 (SFX on Hen egg-white lysozyme, AGIPD detector)	Diffraction	Lysozyme	serial femtosecond crystallography	2020-03-09 01:20:02 +0100	Closed	Good			
0029 (SFX on Hen egg-white lysozyme, AGIPD detector)	Diffraction	Lysozyme	serial femtosecond crystallography	2020-03-09 01:07:51 +0100	Closed	Good			
0027 (SAXS on 50 nm silica, AGIPD detector at MID instrument)	scattering	Silica 50nm	small angle x-ray scattering	2019-09-21 01:12:49 +0200	Closed	Good			
0026 (Time-resolved SAXS on Ni75-11 MLs, DSSC detector at SCS)	SAXS 500kHz // no pump laser	Ni75-11 MLs-b	small angle x-ray scattering	2019-08-23 07:08:02 +0200	Closed	Good			

Direct access to open data, requires enhanced Globus service

Data interoperability: NeXus support

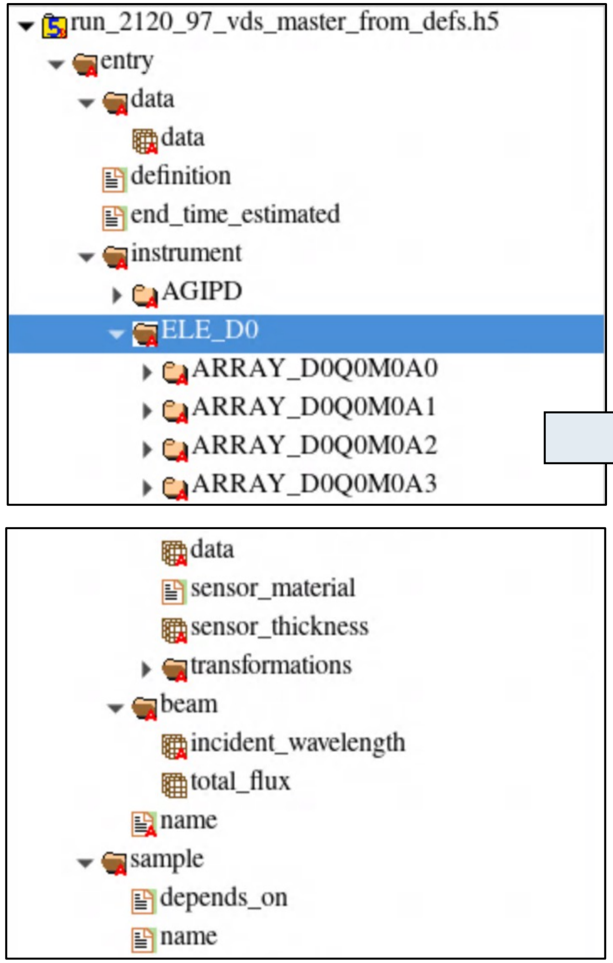


Detector geometry



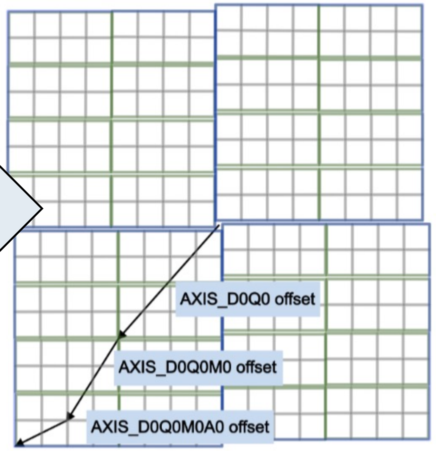
Other compulsory metadata sources

NeXus application definitions



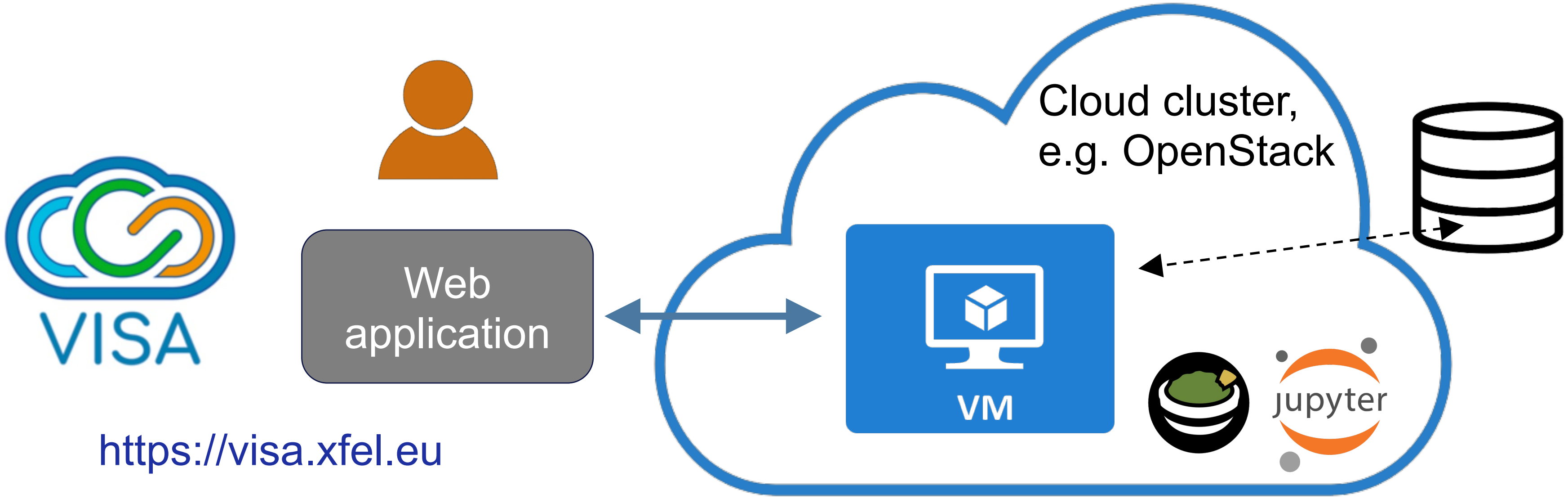
```
run_2120_97_vds_master_from_defs.h5
  entry
    data
      data
    definition
    end_time_estimated
    instrument
      AGIPD
      ELE_D0
        ARRAY_D0Q0M0A0
        ARRAY_D0Q0M0A1
        ARRAY_D0Q0M0A2
        ARRAY_D0Q0M0A3
```

```
        data
        sensor_material
        sensor_thickness
        transformations
      beam
        incident_wavelength
        total_flux
      name
    sample
      depends_on
      name
```



NeXus NxMX standard master file

Reusing open EuXFEL data: analysis in the cloud



https://visa.xfel.eu

- Enables data analysis from anywhere with a web browser, requires no local SW requirements or installations
- Data analysis is performed where the facility data is: no need to download tons of data
- Employs cluster resources with simple and transparent configuration of virtual machines
- Brings Jupyter notebooks and GUI programs with remote desktop under the same roof

Summary and Outlook

- European XFEL data stems from a unique time structure with very high FEL pulse and detector repetition rates and accounts for extreme storage volumes
- Data reduction methods are known and need to be well implemented to automated facility services and anchored in an adequate scientific data policy.
- SFX data offers considerable reduction potential due to low hits rates in typical experimental setups
- Data analysis (incl. re-use) services for users exist – now they have to be expanded for guests interested in open, i. e. post-embargo, data
- To adopt FAIR principles better, developments for catalogue integration to search services, remote/cloud-based data analysis and standards for interoperability are ongoing

Thanks and credits to all colleagues from European XFEL, collaborators of the PaNOSC/ExPaNDS projects, and users – for their work, help and ideas in fostering FAIR science adoption at our facility

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Always FAIRplay!

Thank you for your attention!