

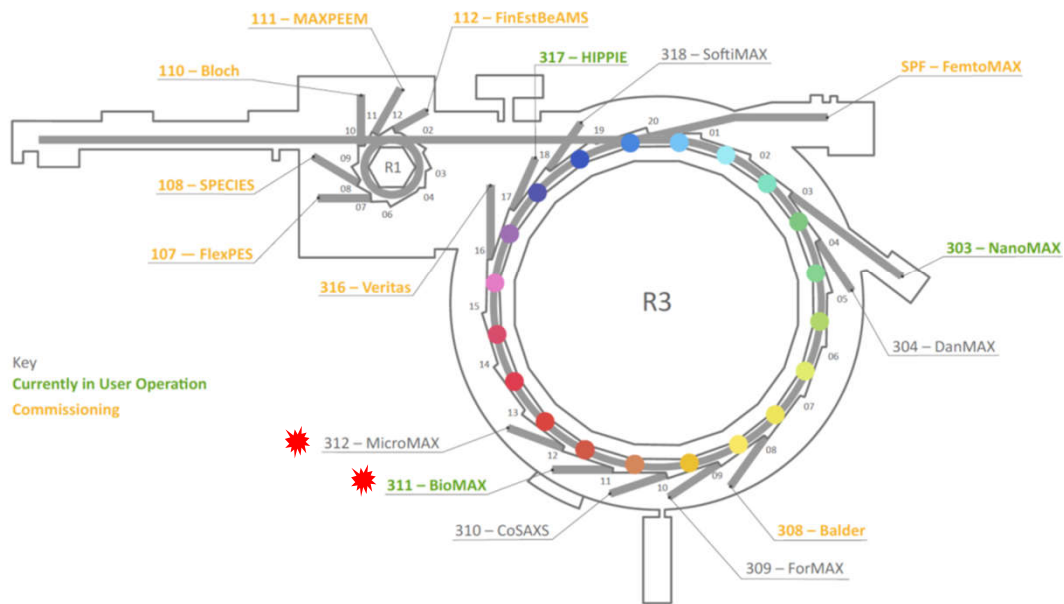


The MX data at MAX IV

Jie Nan

Aug 22, 2020

MX Beamlines at MAX IV



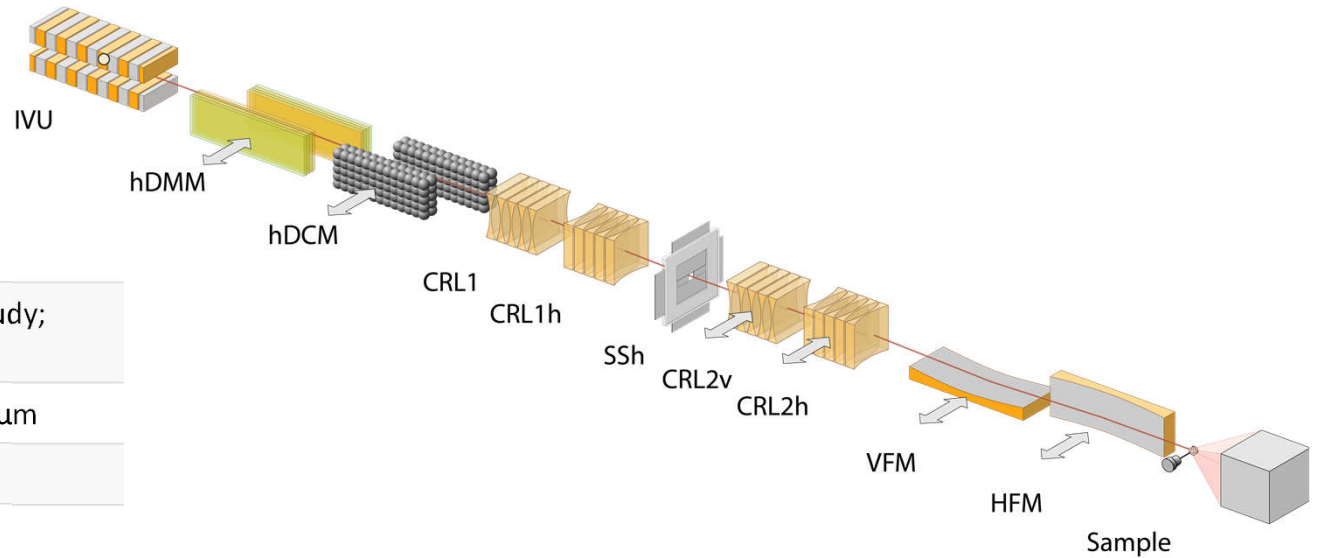
BioMAX – in operation

- In-vacuum undulator
- 5 – 25 keV
- 4×10^{12} ph/s @sample position
(250mA ring current)
- BCU
- MD3 Diffractometer
- Cryojet5, HC-lab and REX
- Amptek fluorescence detector
- **Eiger16M**
- ISARA sample changer



- Since Mid-march 2020, only remote operation due to Covid-19
- Fast data collection and sample exchange, nearly 20 samples per hour

MicroMAX – under construction



Scope	Serial crystallography; time-resolved study; standard rotation collection
Beam Size	Tunable between below 1 μm up to 10 μm
Energy Range	5–20 keV (option of higher energy)
Time Scales	Down to microseconds
User operation	2022

Two detectors

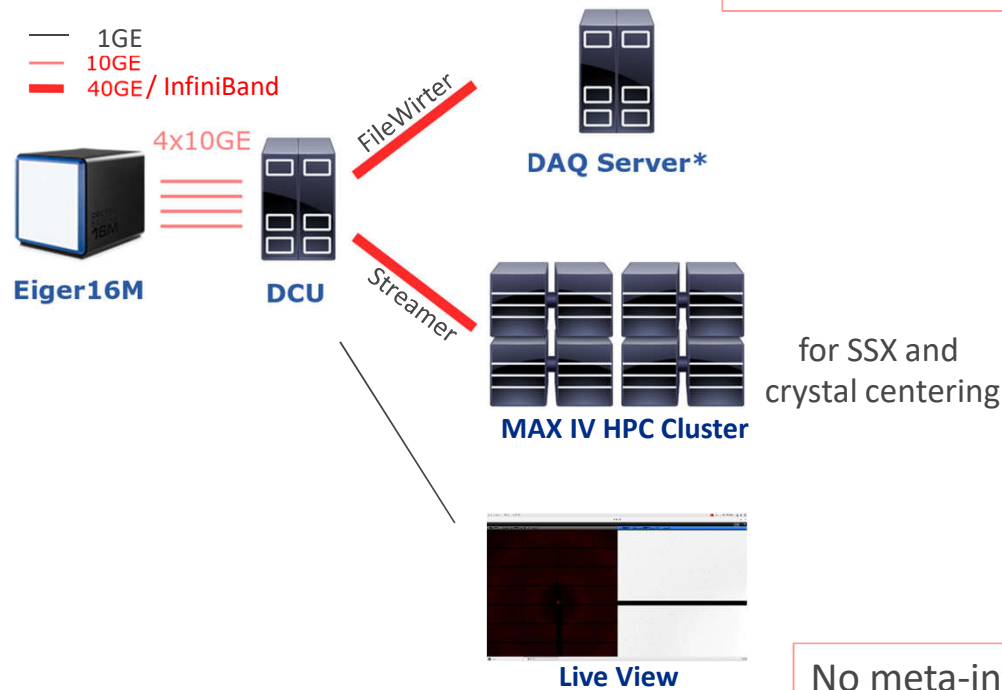
- Jungfrau 4M
- Photon-counting detector

Eiger 16M at BioMAX

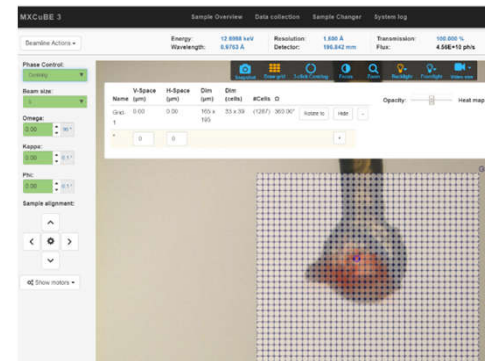
- In operation since Dec. 2016
- Used for both rotation collections as well as SSX (fix-target and injector)
- Filewriter, Streamer and Monitor

Eiger 16M at BioMAX

Fill all relevant entries in master file and add necessary info so that users can (re)process the raw data w/o beamline input files



No meta-info



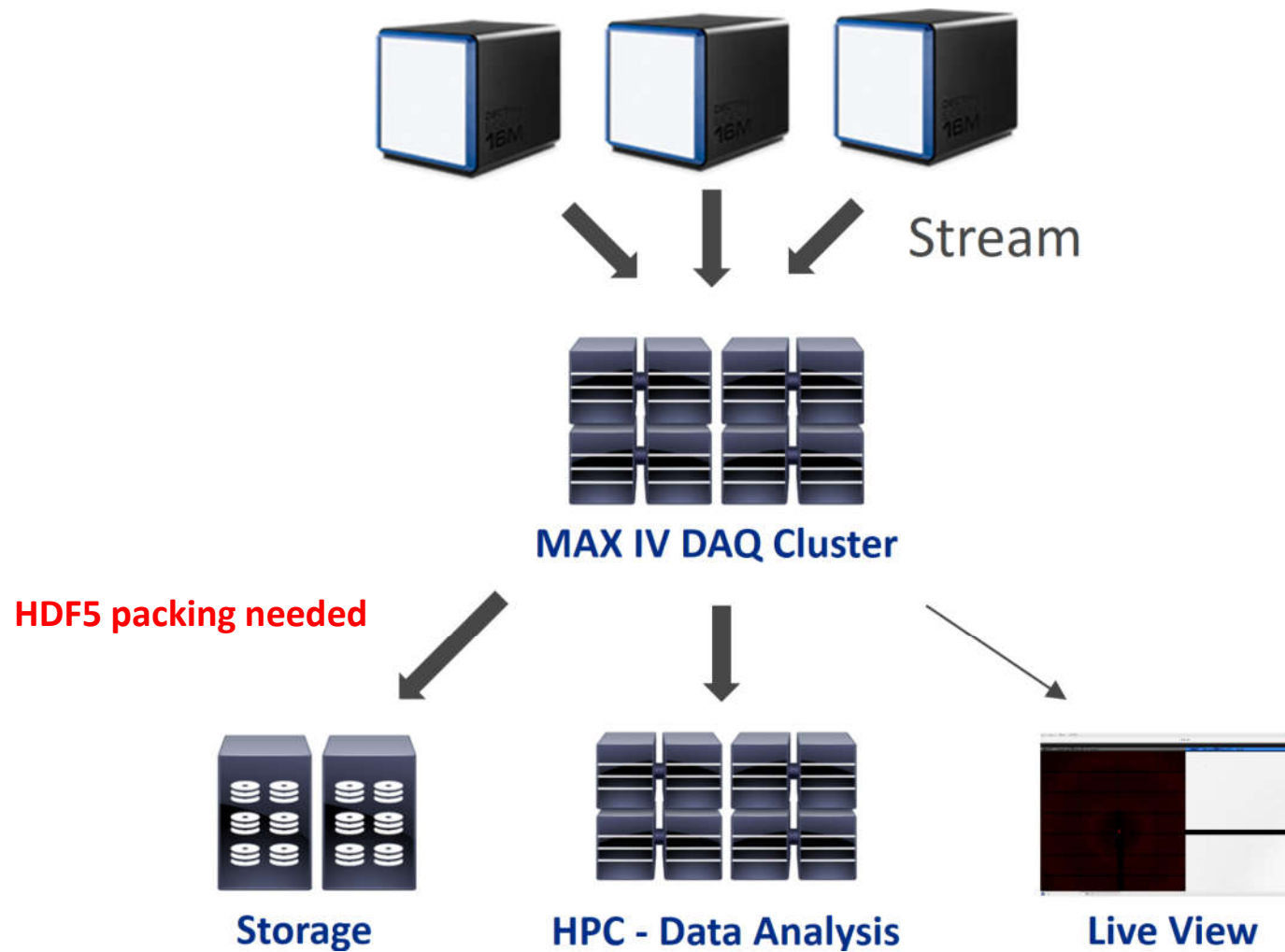
Only crucial meta info for the on-the-fly analysis and feedback to control software, images are discarded after analysis

Current state of the raw image

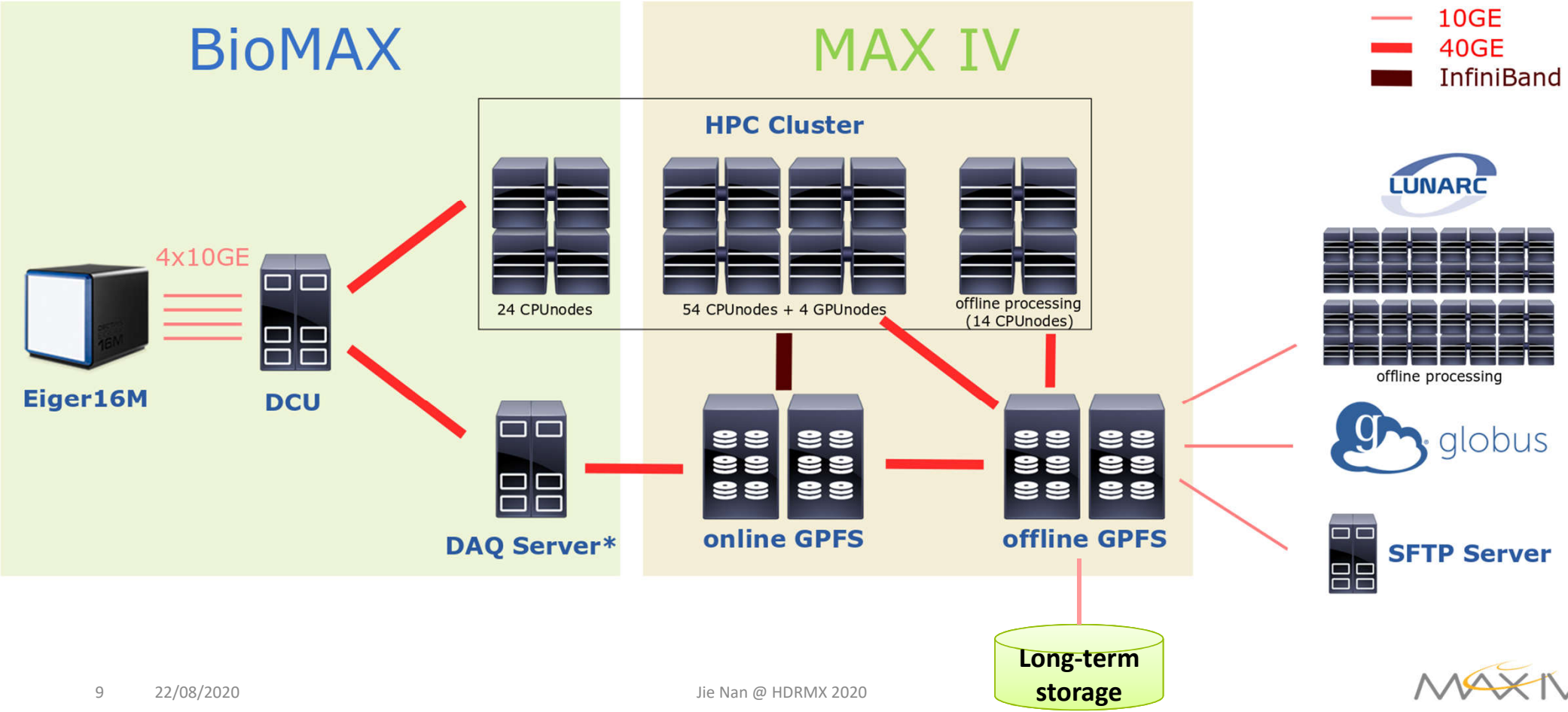
Editing of the master file after data collection

- adding rotation axis, `"/entry/sample/transformations/omega/vector"`
 - adding beamline name, `"/entry/instrument"` (attrs['name'] = `"BioMAX@MAXIV"`)
- } From Day 1 operation
- For characterization collection, modifying `"/entry/sample/goniometer/omega"` and `"/entry/sample/goniometer/omega_end"`, e.x. four images of 0-1, 90-91, 180-181, 270-271 deg from one arm four triggers, in the original master file, they are 0-1, 1-2, 2-3, 3-4 deg

Generic framework at MAX IV – under development



IT infrastructure for BioMAX

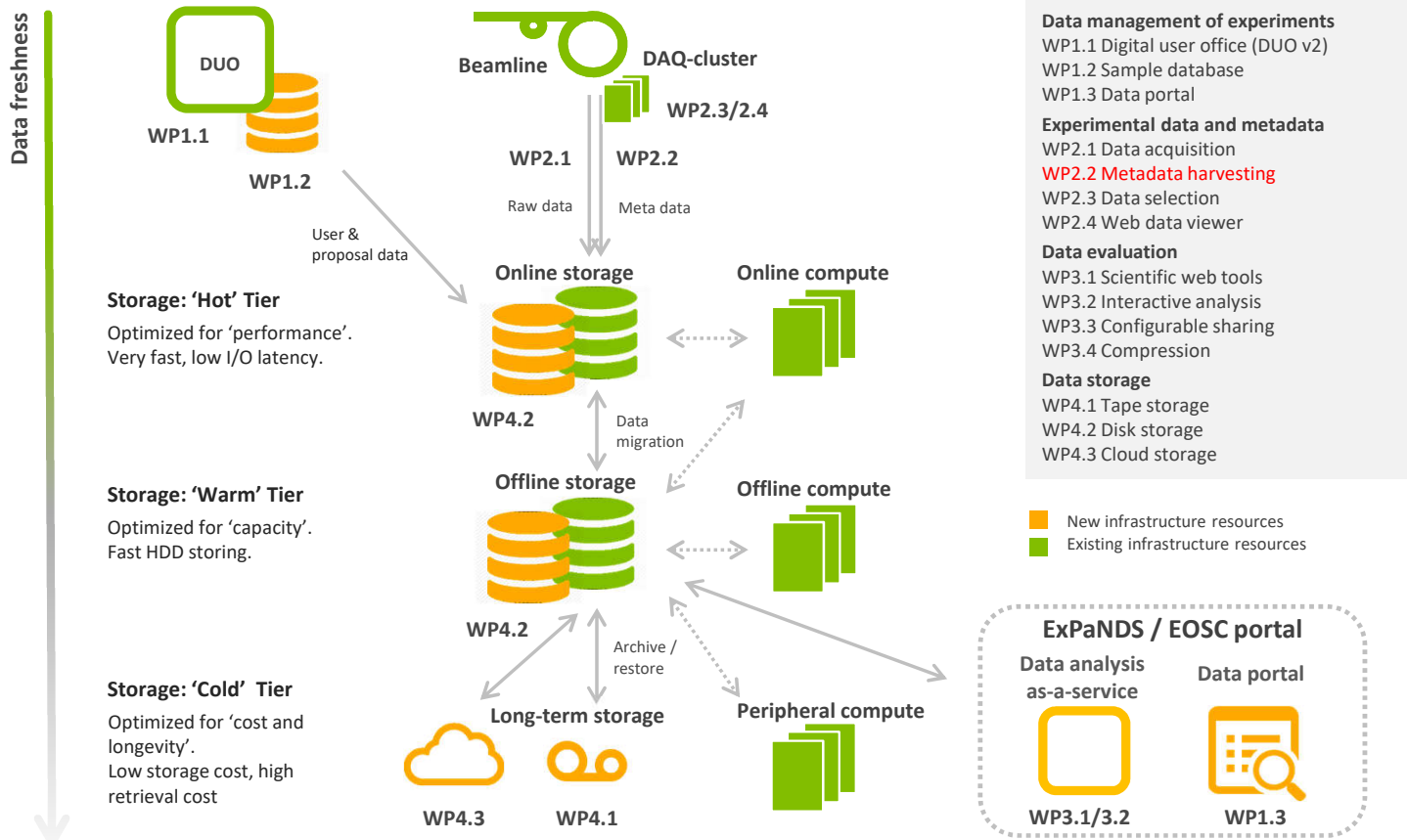


DataSTaMP at MAX IV

- DataSTaMP - Data Storage and Management Project (2019-2023)
- To improve the data storage infrastructure and the data management services at MAX IV.
- Aims at supplying FAIR data services to the MAX IV user community and ensure data taken at MAX IV can be stored long-term.

*Knut and Alice
Wallenberg
Foundation*

Research lifecycle



- Data management of experiments**
- WP1.1 Digital user office (DUO v2)
 - WP1.2 Sample database
 - WP1.3 Data portal
- Experimental data and metadata**
- WP2.1 Data acquisition
 - WP2.2 Metadata harvesting
 - WP2.3 Data selection
 - WP2.4 Web data viewer
- Data evaluation**
- WP3.1 Scientific web tools
 - WP3.2 Interactive analysis
 - WP3.3 Configurable sharing
 - WP3.4 Compression
- Data storage**
- WP4.1 Tape storage
 - WP4.2 Disk storage
 - WP4.3 Cloud storage

From Magnus Klingberg

Future plan - Gold Standard

Goal:

- Short term, add the missing required information, e.x. Total_flux, facility
- Long term, comply to FAIR

Questions:

- total_flux, flux at sample position with or without attenuation? The example from DLS <https://zenodo.org/record/3385862>, have both /entry/beam/flux and /entry/sample/flux
- Missing entry, sample image, translation (e.x. Helical scan)
- Interleave, inverse collection using multi-triggers, repacking or VDS?

Acknowledgements

MX group

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Magnus Klingberg
Thomas Eriksson
Zdenek Matej

Many others from MAX IV

HDRMX community!!