MAX IV
Bliss Workshop@DESY

Vincent Hardion, 22/11/2023

MAX IV

- Experimental Control System at MAX IV
- Detector and Data Processing
- Bliss Context at MAX IV
- Pro/Cons of Bliss at MAX IV Laboratory
- Conclusion

Experimental System at MAX IV

HARD X-RAY: Mainly Command Line Interface
Almost exclusively Continuous/Fly Scan:
- ascan, meshscan, custom macro
- Time Resolved
- Pulse based
- Tomography
- Energy scan

- Step Scan: mostly for alignment

SOFT X-RAY: High need in GUI
Almost exclusively Step by Step Scan:
- Scienta (WIP)
- Prodigy (WIP)
- Elmitec microscope

Continuous Scan
- Energy Scan
- NEXAFS

HARDWARE: more and more high-level responsibility
Synchronisation Continuous/Fly Scan:
- PandaBox
- ACS

Motors: Handle High level parameters/trajectories
- Icepap (standard)
- Piezo
- ACS

SOFTWARE:
Orchestration and macro management:
- Sardana

Data acquisition:
- Streaming to a dedicated compute cluster
- On-the-fly analysis(Azimuthal, ToT), Live view
- Hdf5
- Meta data: SciCAT

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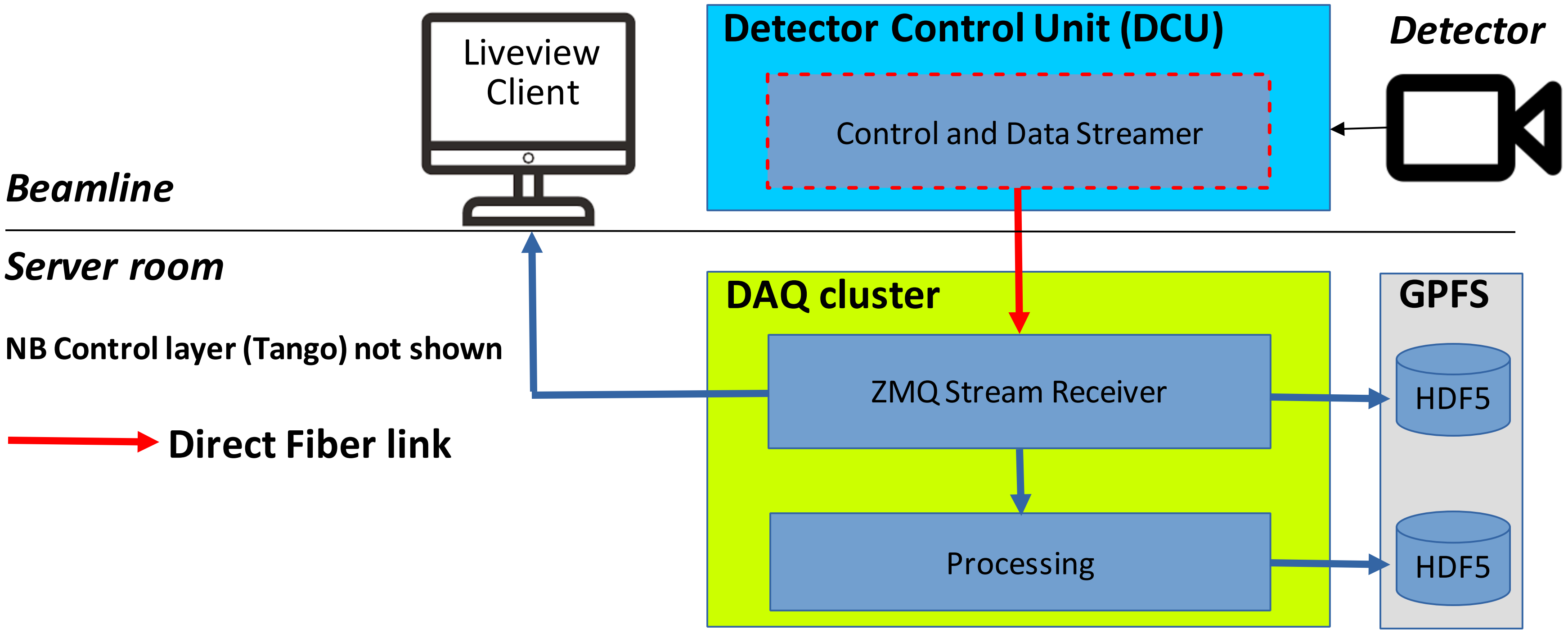
DAQ data flow scheme



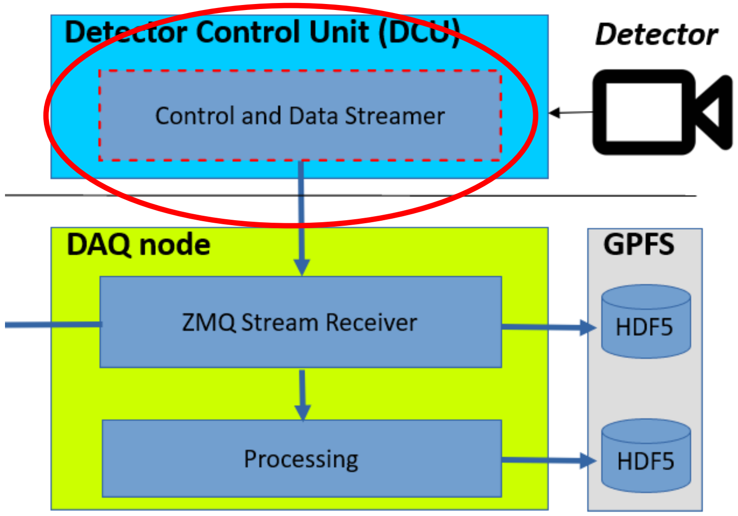
Courtesy of Paul Bell, MAX IV

DCU streamer part

- Detector interfaces to DCU in hardware specific way (fibre, CameraLink, USB...)
- Specific software layer written for that detector:

  Gets frames, streams them off the DCU to the DAQ cluster

  (Won't talk about control)



- For a new detector, this is where most of the work must be done

Courtesy of Paul Bell, MAX IV

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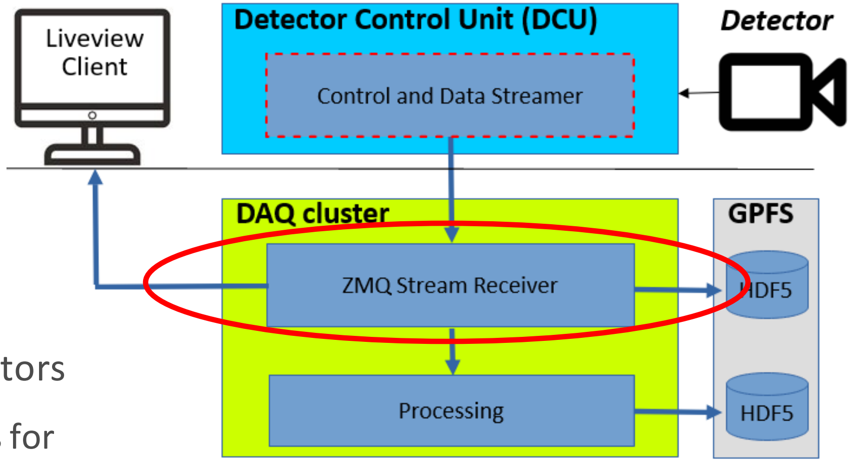
DAQ receiver part

- DAQ cluster managed by kubernetes
- Receiver = 1 process in 1 container in 1 pod
- Writes all frames to disk (hdf5 files in GPFS)



Internal Project Work Jan - June 2023:

- One standard receiver now handles all detectors
- With IT Infra – fast to deploy the Receiver in k8s for any new detector
- Means live view is common, hdf5 writing is common

cosaxs-eiger

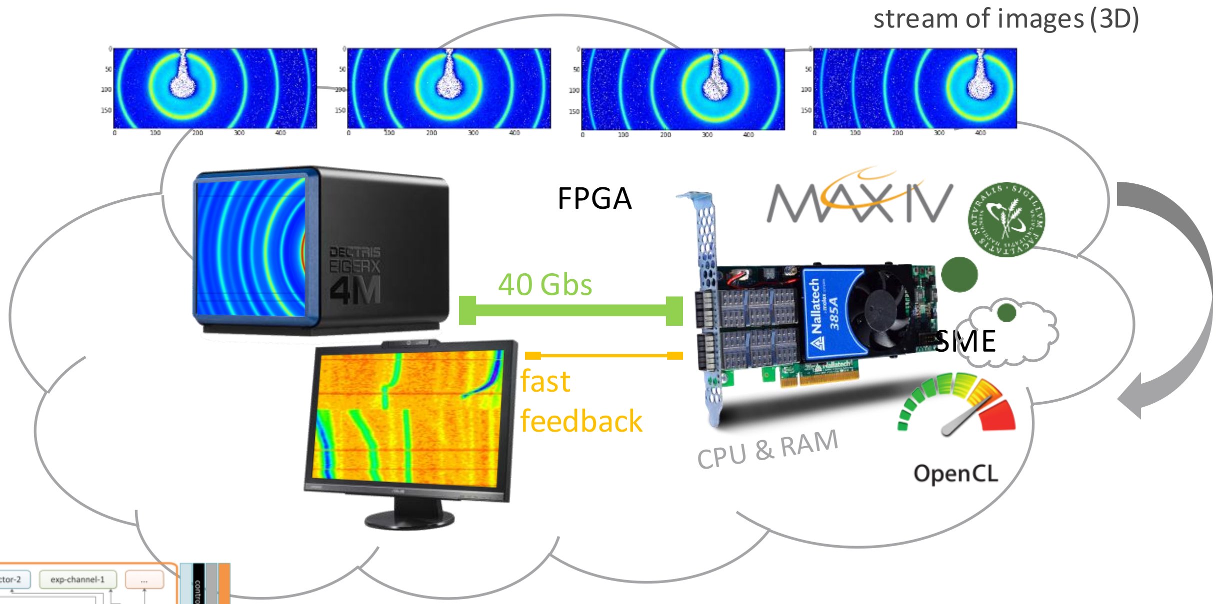
Deployments

Redeploy | Download YAML | Delete | Create

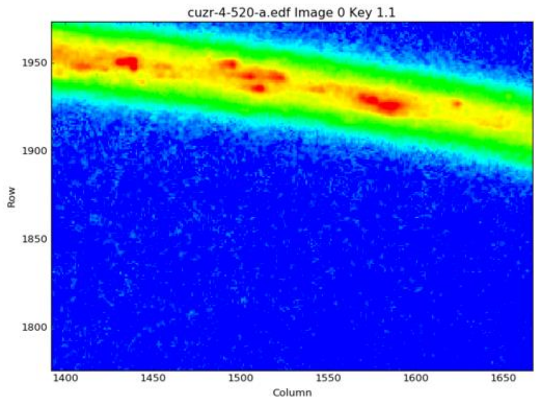
State	Name	Namespace	Image	Ready	Up To Date	Available	Restarts	Age	Health
Active	coasxs-eiger-azint	cosaxs-eiger	harbor.maxiv.lu.se/daq/azint-pipeline:2.0.1	1/1	1	1	0	200 days	
Active	coasxs-eiger-ctl	cosaxs-eiger	harbor.maxiv.lu.se/daq/kubernetes/pipeline-ctl:0.2.0	1/1	1	1	0	200 days	
Active	coasxs-eiger-daq	cosaxs-eiger	harbor.maxiv.lu.se/daq/streaming-receiver:3.3.0	1/1	1	1	0	200 days	

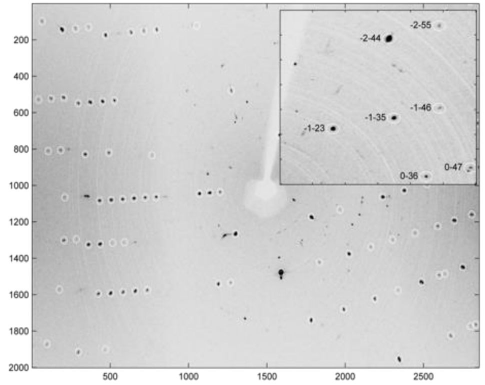
Courtesy of Paul Bell, MAX IV

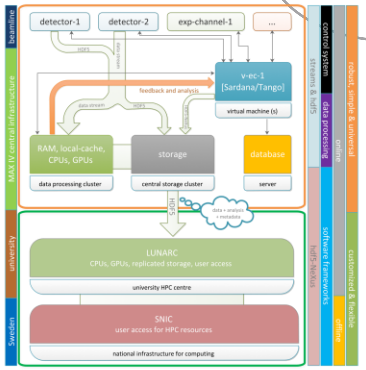
On the fly Feedback



- roi couting
- diffraction spot finding
- frame filtering
- image corrections (dark/flat field)
- decompression
- segmentation
- phasing
- tomographic reconstructions
- ML & AI prediction



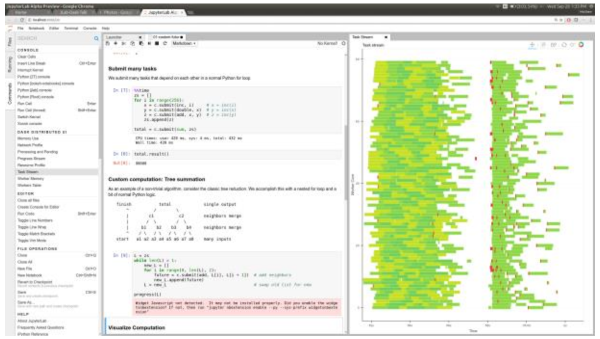




The MAX IV imaging concept
Matěj et al. ASCI 2017

DASK

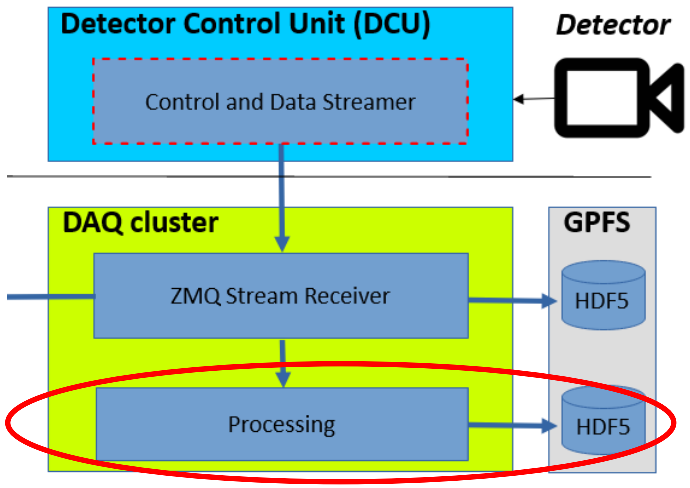
kubernetes

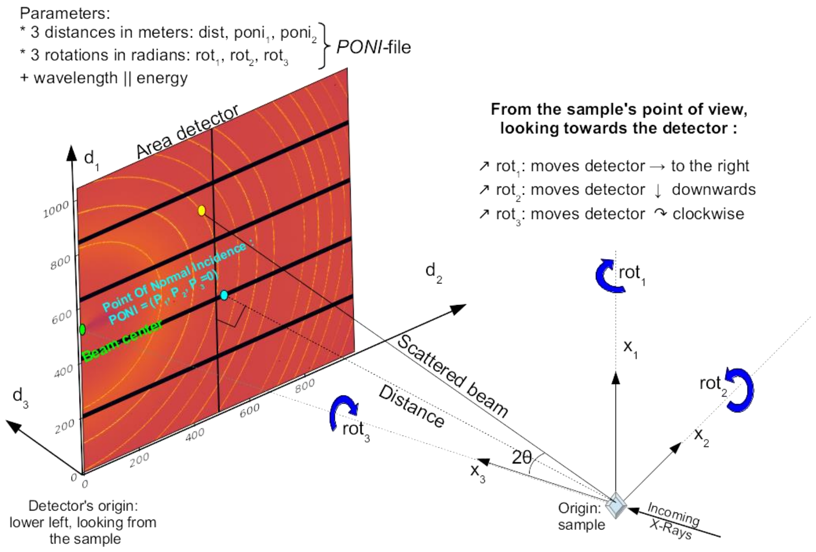


Courtesy of Zdenek Matej, MAX IV

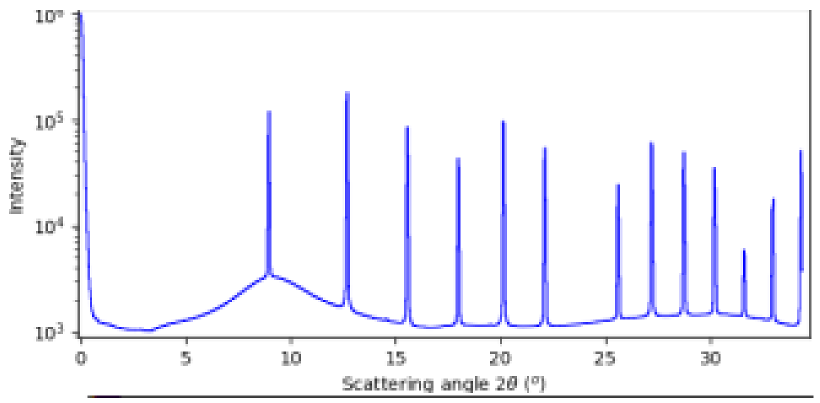
Processing part

- Processing step today often means azimuthal integration
- Provided by "azint" alogorithm (Clemens Weninger)
- Runs at ForMAX, CoSAXS, DanMAX, FemtoMAX, NanoMAX, Balder





- ***Data reduction: 2D -> 1D***



Courtesy of Paul Bell, MAX IV

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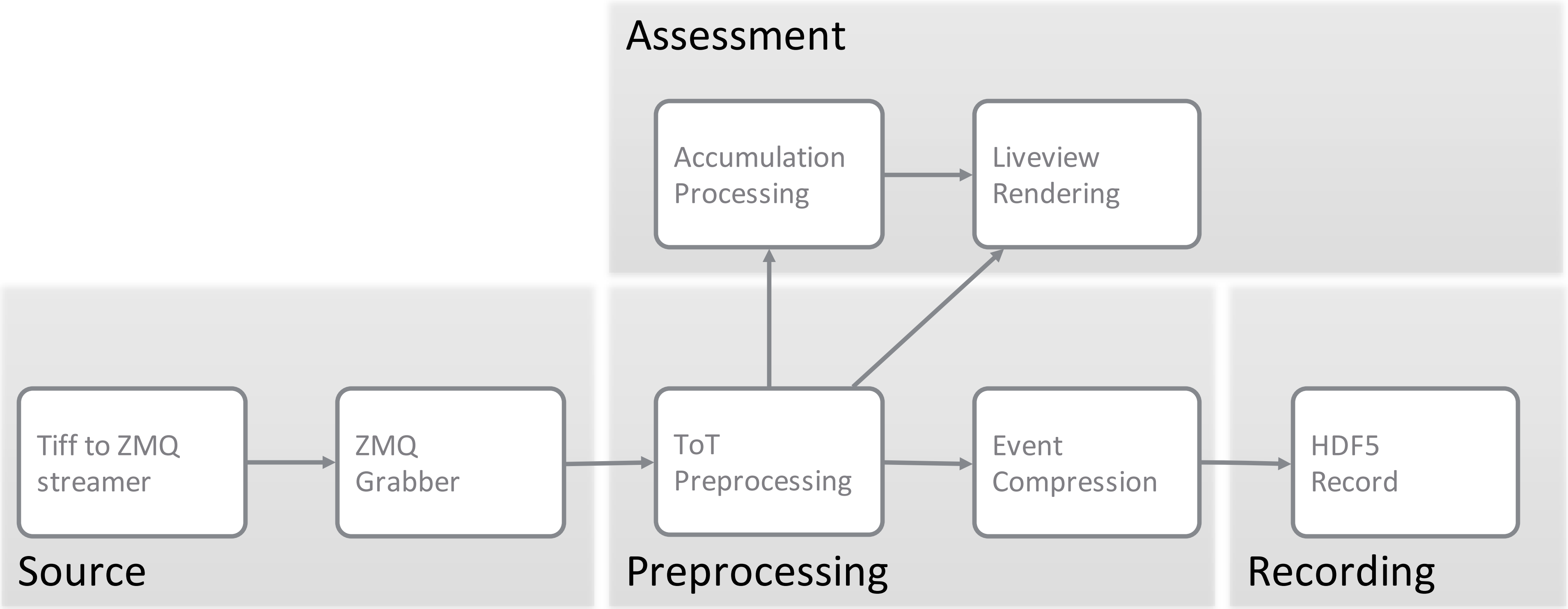
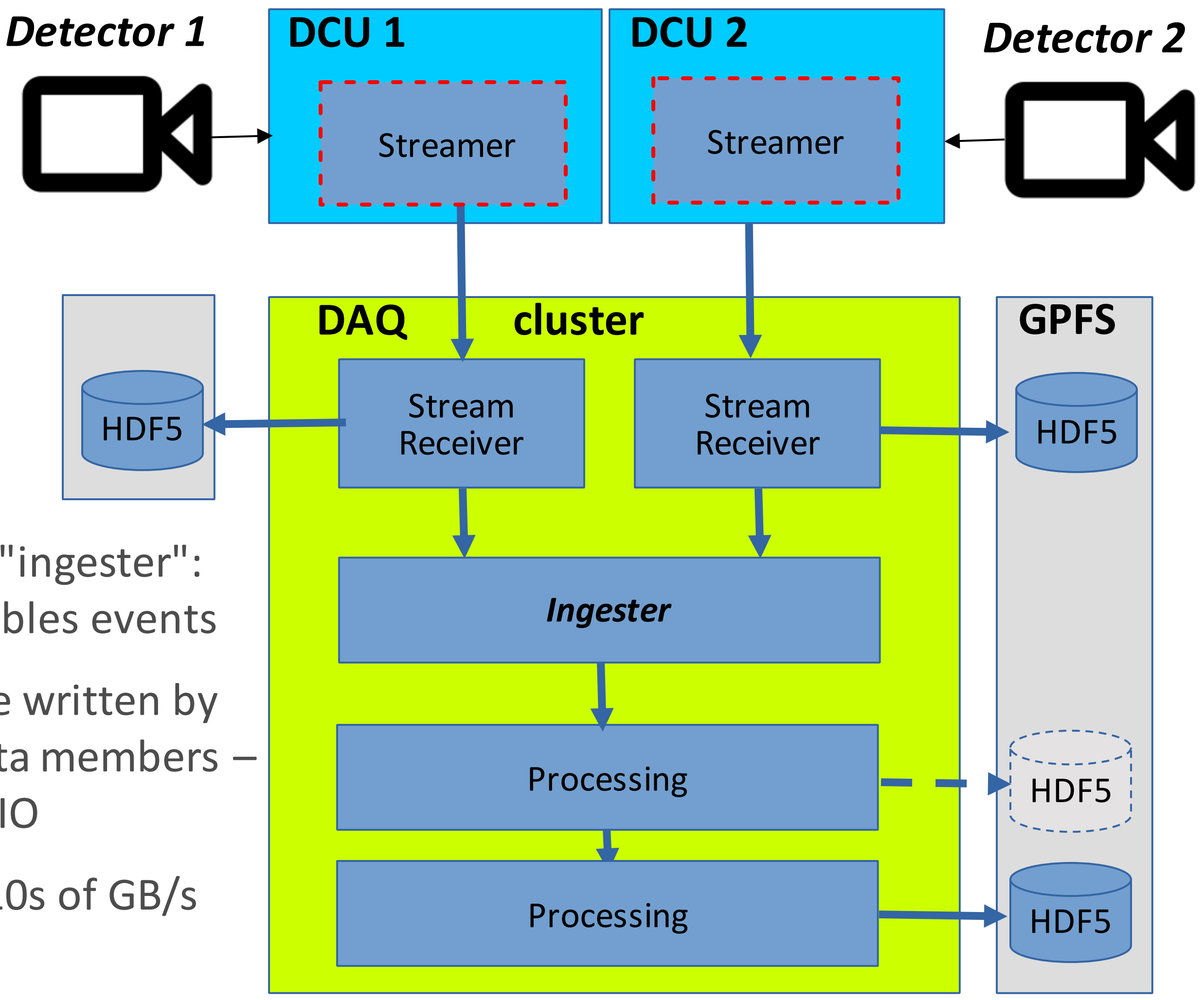
Femtomax Scattering pipeline



Pipelines machinery for general case

Two requirements not addressed in simple scheme:

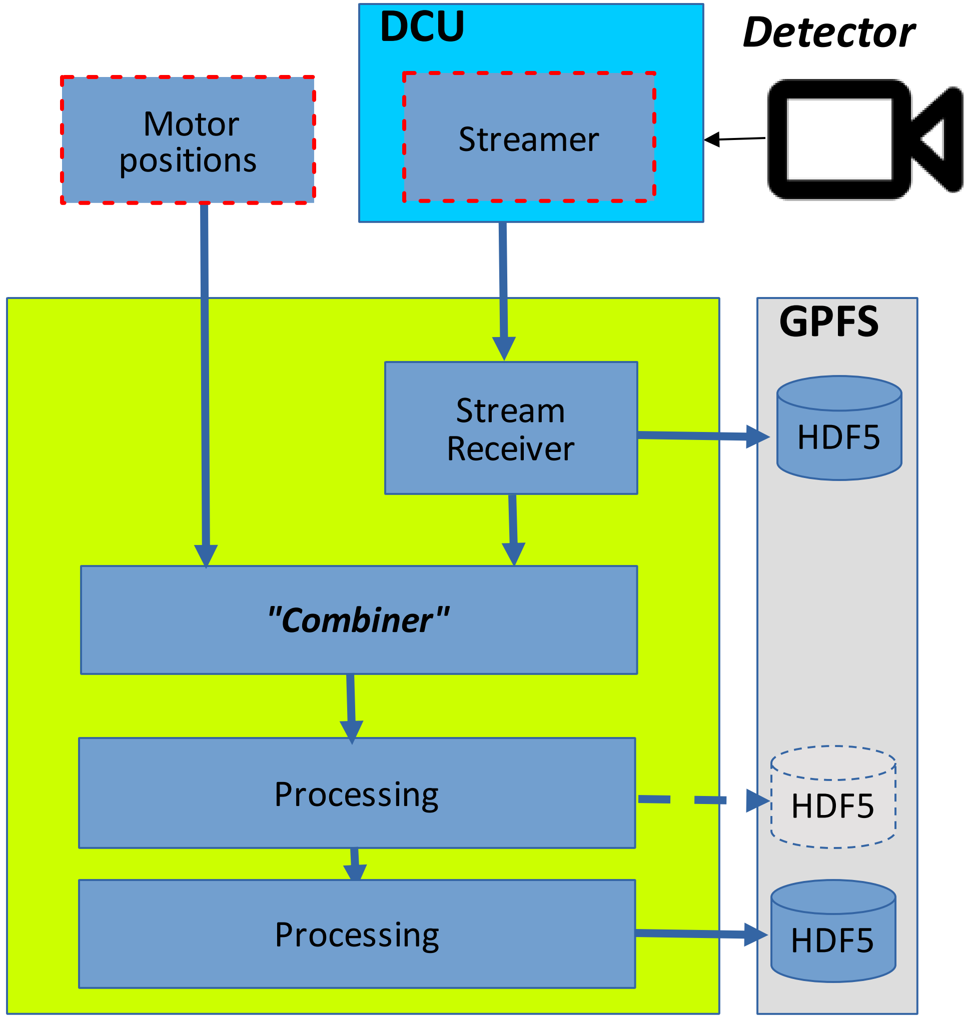
- Processing may have several steps
- Processing may take input from multiple sources
- New component - the "ingester": matches inputs, assembles events
- Algorithms can then be written by scientists/other Sci Data members – standard interface for IO
- Scaled for few kHz or 10s of GB/s using the power of k8s
- (When confident could save only processed data)



Courtesy of Paul Bell, MAX IV

FemtoMAX case today

One day could allow closed loop feedback where the scan parameters are adjusted based on collected data (eg. Scan area of interest) !



Courtesy of Paul Bell, MAX IV

Context for Bliss workshop

- Project 2023: Evaluation of the Experiment Control System
  - Sardana, Bluesky, Bliss, Contrast, …

- Bliss: just started evaluation
  - First overview
  - Test of Daiquiri in 2021 (after ICALEPCS)
    - Try (quickly) to connect to sardana without success

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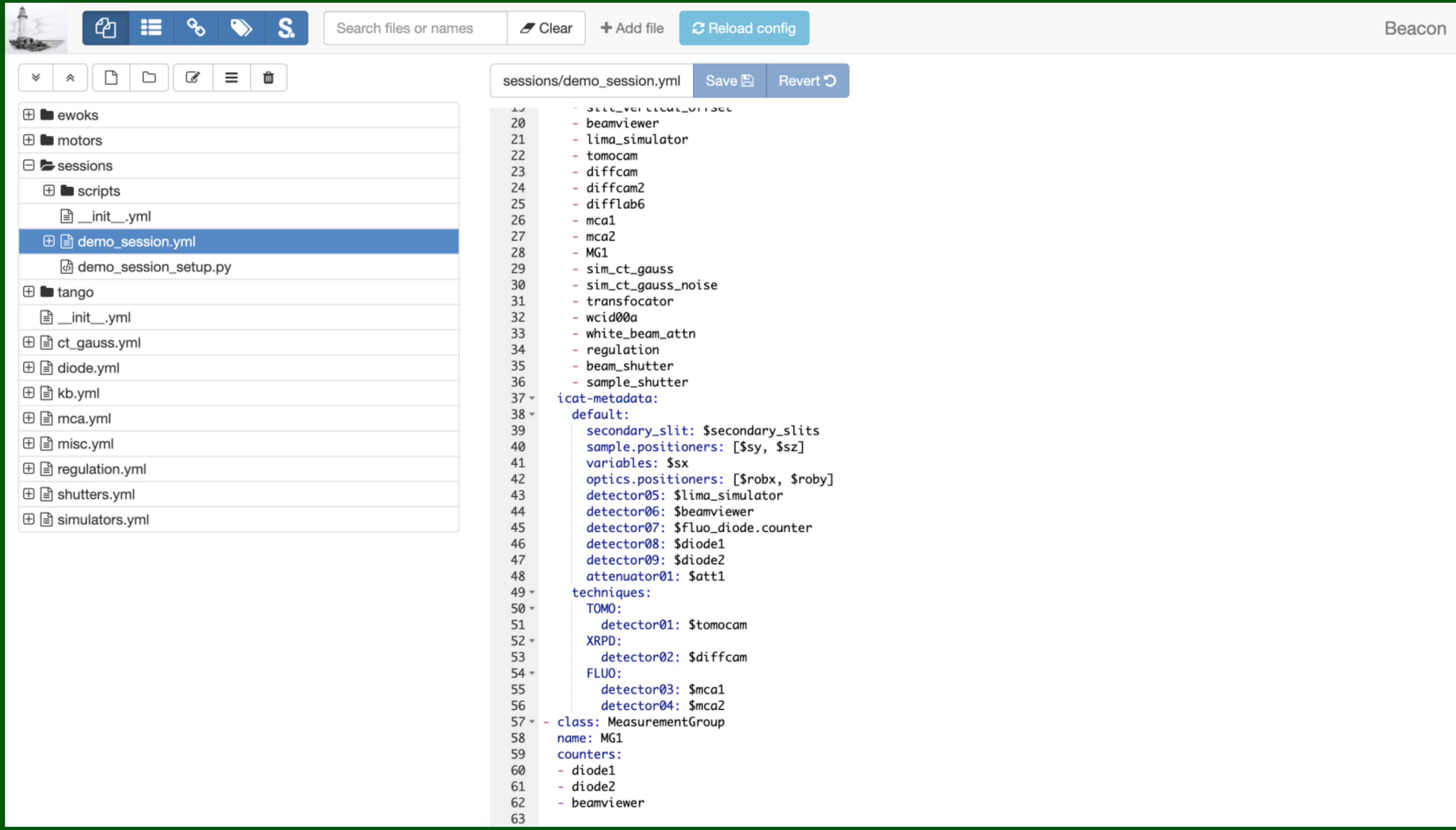
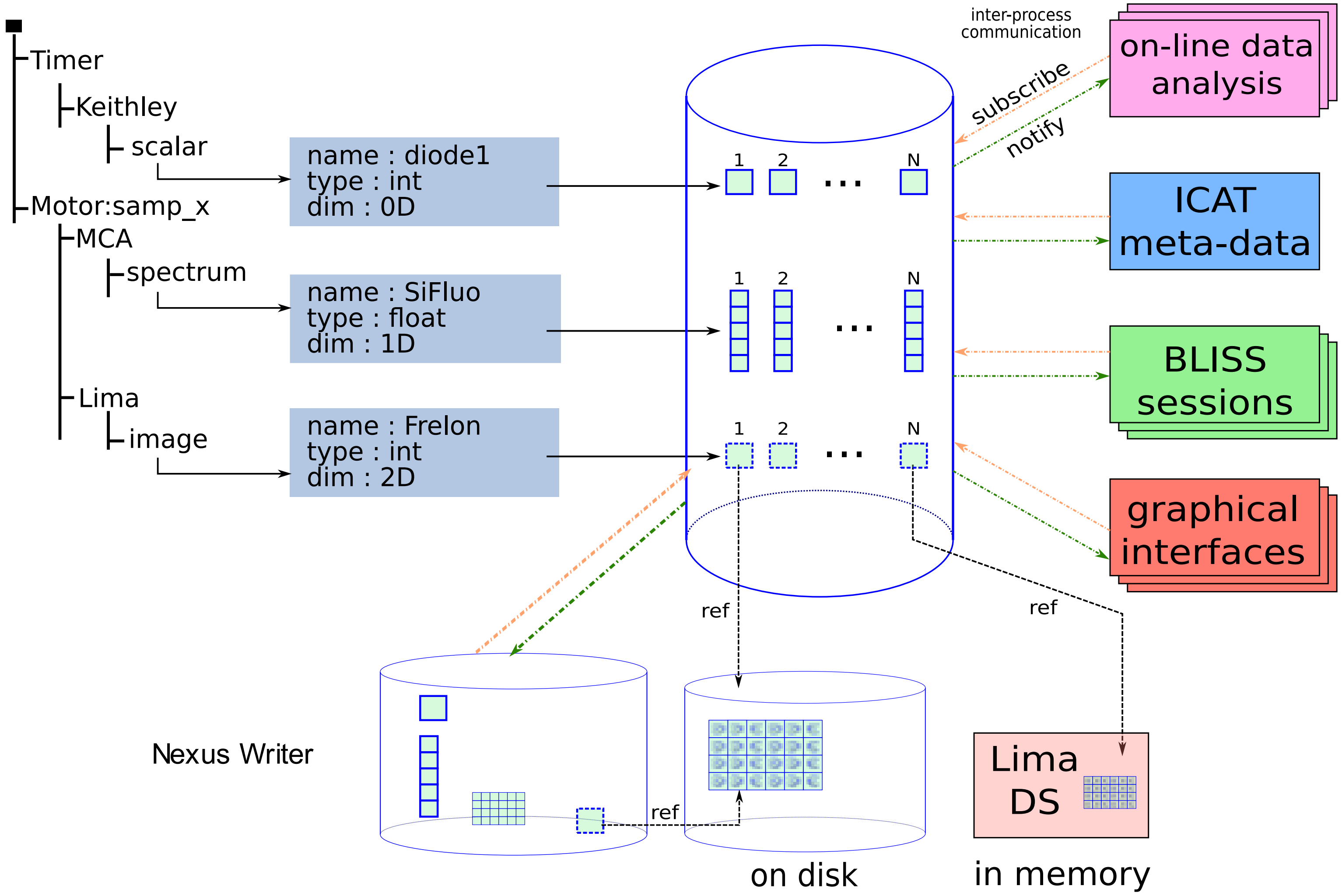
Scan configuration

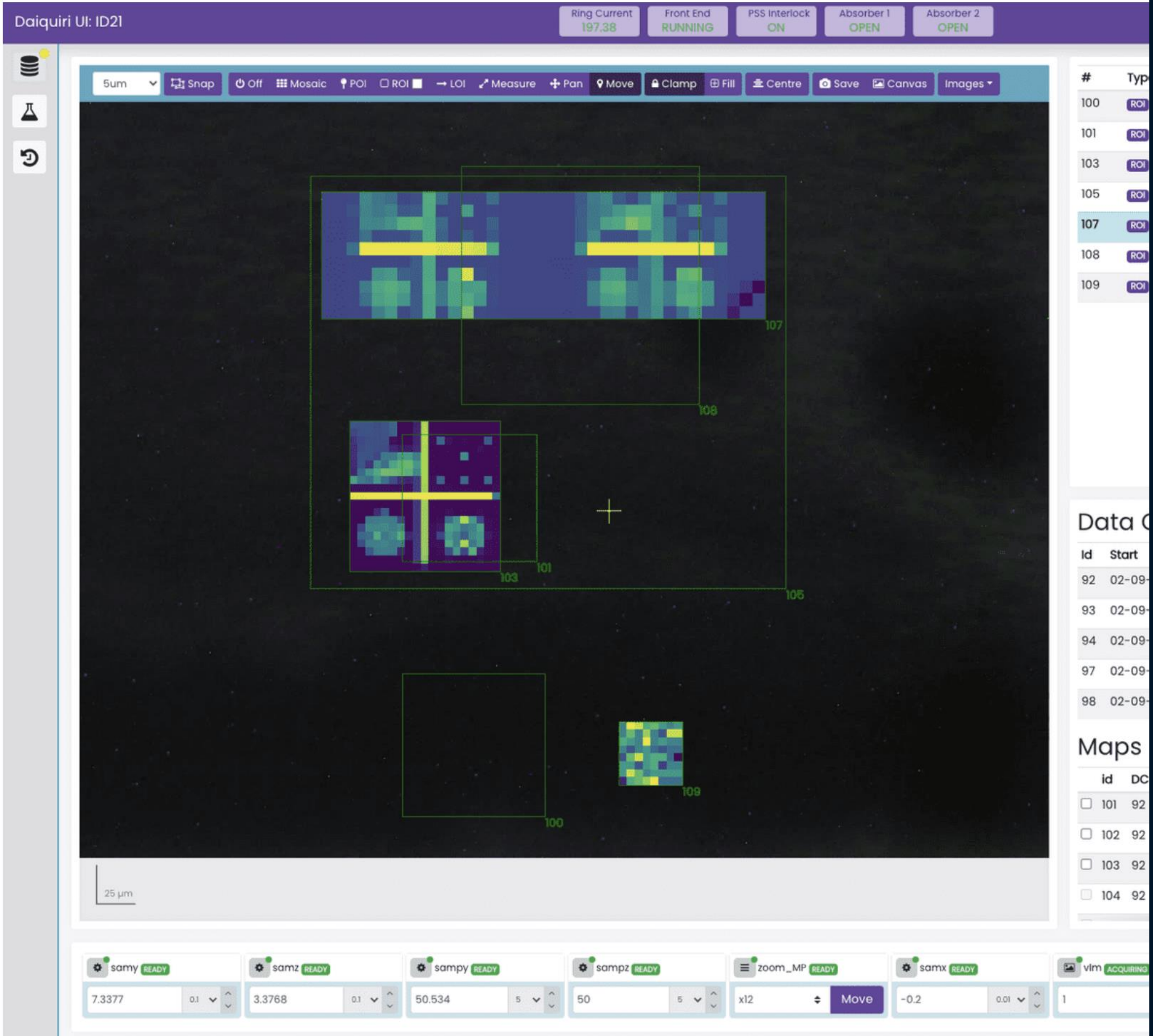
- Full configuration management
- Session/Technic
- metadata
- Include/exclude instruments
- Macro/hook



Bliss data

- Independent Agent => not blocking the scan
- Possibility to easily distribute the data to different consumer





UI Mapping

- Microscopy UI
- 2D Mapping management
- Sample management

Data processing

- Online data processing pipeline with **Ewoks**
- Live Feedback to Experiment Control System

research papers

JOURNAL OF SYNCHROTRON RADIATION

ISSN 1600-5775

Closing the loop: autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments

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Received 21 June 2023
Accepted 26 August 2023

Edited by U. Jeng, NSRRC, Taiwan

Keywords: machine learning; reflectometry; autonomous experiments; beamline control; XRR; closed-loop control.

Supporting information: this article has supporting information at journals.iucr.org/s

Recently, there has been significant interest in applying machine-learning (ML) techniques to the automated analysis of X-ray scattering experiments, due to the increasing speed and size at which datasets are generated. ML-based analysis presents an important opportunity to establish a closed-loop feedback system, enabling monitoring and real-time decision-making based on online data analysis. In this study, the incorporation of a combined one-dimensional convolutional neural network (CNN) and multilayer perceptron that is trained to extract physical thin-film parameters (thickness, density, roughness) and capable of taking into account prior knowledge is described. ML-based online analysis results are processed in a closed-loop workflow for X-ray reflectometry (XRR), using the growth of organic thin films as an example. Our focus lies on the beamline integration of ML-based online data analysis and closed-loop feedback. Our data demonstrate the accuracy and robustness of ML methods for analyzing XRR curves and Bragg reflections and its autonomous control over a vacuum deposition setup.

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Bliss at MAX IV? (As wip of 11/2023)

PRO:
- Integrated framework as Sardana
- Modern design
- Documentation, cheatsheet
- Configuration management + web interface
- Data handling Based on broker
- Concept similar as Sardana
- Notion of Proposal/Collection/DataSet
- Pythonic
- Better error handling

Challenges:
- Community
- Specific Integration to ESRF service: Lima, ICAT, logbook
- Integration with our system: zmq streaming, SciCAT
- Limited UI framework
- Multiple synchronisation schema
- Hardware scanning orchestration
- Not Simple as Bluesky
- Sharing session with TMUX
- CLI with"(" ;-)

- TO BE CHECKED:
- Control of pseudo motor (case undulator)
- Run just as library (Bluesky-like)
- FlyScan

Conclusion

- Experiment System at MAX IV:
  - Continuous/FLY Scan with more HW
  - Analysers with more UI
- Data Handling and Processing
  - ZMQ
  - Kubernetes cluster
- Next steps
  - Detailed evaluation at MAX IV
  - If possible in-situ

Question?

Question Everything (Nullius in verba), Dunk