



| The European Synchrotron

# BLISS SOFTWARE ECOSYSTEM



## Outline

- **What scientists need**
- **What we have**
- **What can be exported**

Jens Meyer on behalf of the ESRF Beamline Control Unit

# WHAT THE SCIENTIST NEEDS

Experiment automation

Data acquisition

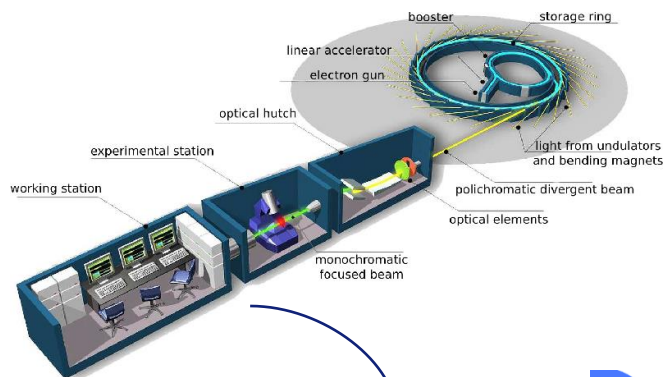
Data and meta data organization

Data reduction

Data analysis



Software: EVERYWHERE from photons to paper publication



RESEARCH ARTICLE  
ADVANCED SCIENCE NEWS  
www.advancedsciencenews.com

## Spatially Resolved Dynamics of Cobalt Color Centers in ZnO Nanowires

Christian T. Plass,<sup>1</sup> Valentino Bonino, Maurizio Ritzer, Lukas R. Jäger, Vicente Rey-Bastuko, Martin Heffernann, Jaime Segura-Ruiz, Crema Martínez-Crisdo, and Carsten Römig

The dynamics of color centers, being a promising quantum technology, is strongly dependent on the local environment. A synergistic approach of X-ray Fluorescence analysis and X-ray excited optical luminescence (XEOL) using a hard X-ray nanoprobe is applied. The simultaneous acquisition provides insights into compositional and functional variations at the nanoscale, demonstrating the extraordinary capabilities of these combined techniques. The findings on cobalt-doped zinc oxide nanowires show an anticorrelation between the hard-edge oxidation of the zinc oxide host and the intra-lattice luminescence, indicating two competing recombination paths. Moreover, time-resolved XEOL measurements reveal two exponential decays of the cobalt luminescence. The fast and steady observed ones can be attributed to a recombination cascade within the cobalt sites, resulting from direct excitation. Thus, this opens a new fast timescale for potential devices based on cobalt color centers in ZnO nanowires by photonic circuits.

**1. Introduction**  
Color centers in semiconductors have gained enormous importance for quantum technologies [1]. They provide peculiar properties with relevance reported in the last 20 years [2]. These were observed in several material systems [3] as the generation of single photons and deterministic bit operations [4]. Single molecules [5] or small particles [6] exhibit intrinsically [7] or external [8] quantum entanglement [9]. A promising material with tunable properties for device realizations is based on zinc oxide in zinc oxide (ZnO) [10]. Color centers in ZnO can be achieved by doping it with rare earth elements or transition metals, such as copper, nickel, iron, or cobalt [11]. By optically excitation, cobalt color centers are ionized and the resulting free electrons recombine with the photo-generated carriers. Additionally, the presence of oxygen provides an efficient recombination channel, because transition provides nonspontaneous as well as a route for the entire photon.

**2. Investigation of photophysical dynamics, with respect to the local environment, of ZnO nanowires.**  
In this study, high spatial resolution spectrometer-based XEOL measurements were used to evaluate how the carrier dynamics and the luminescence is influenced by the structural composition and

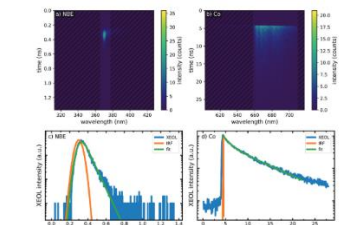
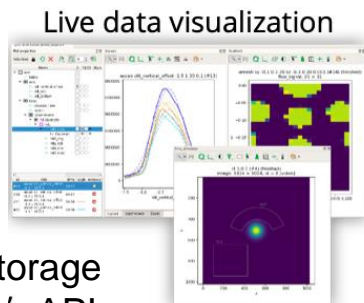
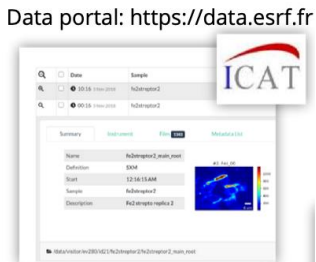
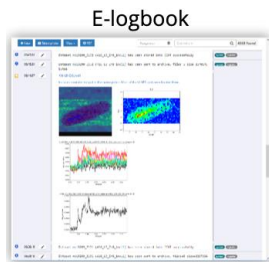


Figure 8. Time-resolved XEOL measurements of single ZnO nanowires at position 1 (indicated in Figure 2a, blue) with the main carrier, spatially resolved near the tip of the ZnO:Co nanowire and ZnO:Co nanowires. XEOL spectral intensity along the wavelength axis within the marked range of the ZnO:Co nanowire and of the ZnO nanowire. The data, the instrument response function, and the resulting fit are shown.

## The ESRF Software Ecosystem



In memory storage and streaming API

On- and offline data analysis workflows

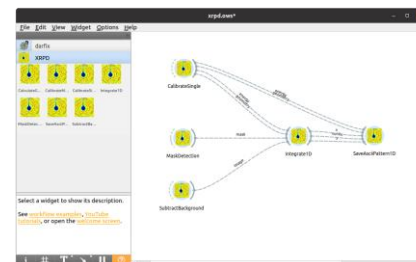
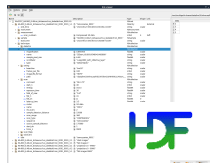
Experiment scripts, user sequences



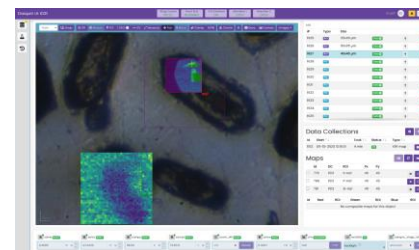
Sequencing and acquisition



File saving



Experiment GUIs



Sample tracking

Status	Updated at	Updated by	Comments
⚠️ NOT BACK TO STOCK	2022-07-27 13:45 GMT	255278	
⚠️ BACK IN STOCK	2022-07-27 13:45 GMT	255278	
⚠️ BEWARE	2022-07-27 13:44 GMT	255278	
⚠️ SPIKES	2022-07-27 13:43 GMT	255278	
⚠️ SICK	2022-07-27 13:43 GMT	255278	
⚠️ APPROVED	2022-07-27 13:43 GMT	255278	
⚠️ READY FOR SAFETY CHECK	2022-07-27 13:22 GMT	255278	
⚠️ NO RESULTS	2022-07-27 13:21 GMT	255278	
⚠️ CREATED	2022-07-27 13:20 GMT	255278	

Experiment automation



Detector integration



## Software modules around BLISS

### Base Layer:

- TANGO: The distributes control system
- HKL library: Diffractometer library from F.Picard, Soleil
- LIMA 1+2: 2D detectors image acquisition library, exported as Tango server
- MOSCA: 1D detectors acquisition library, exported as a Tango Server
- FSCAN: Continuous scan library for BLISS based on ESRF synchronization hardware

### Administrative Layer:

- Sample Tracking: Tracking of samples send from user institutes. Sample identification for automation with sample changers.
- Data Portal: Registration of all data sets and their meta data acquired for an experiment. BLISS pushes the necessary data to ICAT. Archiving and reloading of data sets. User interface to acquired data.
- E-logbook: Logbook attached to every experiment. Can be filled automatically by BLISS or manually.

## Software modules around BLISS

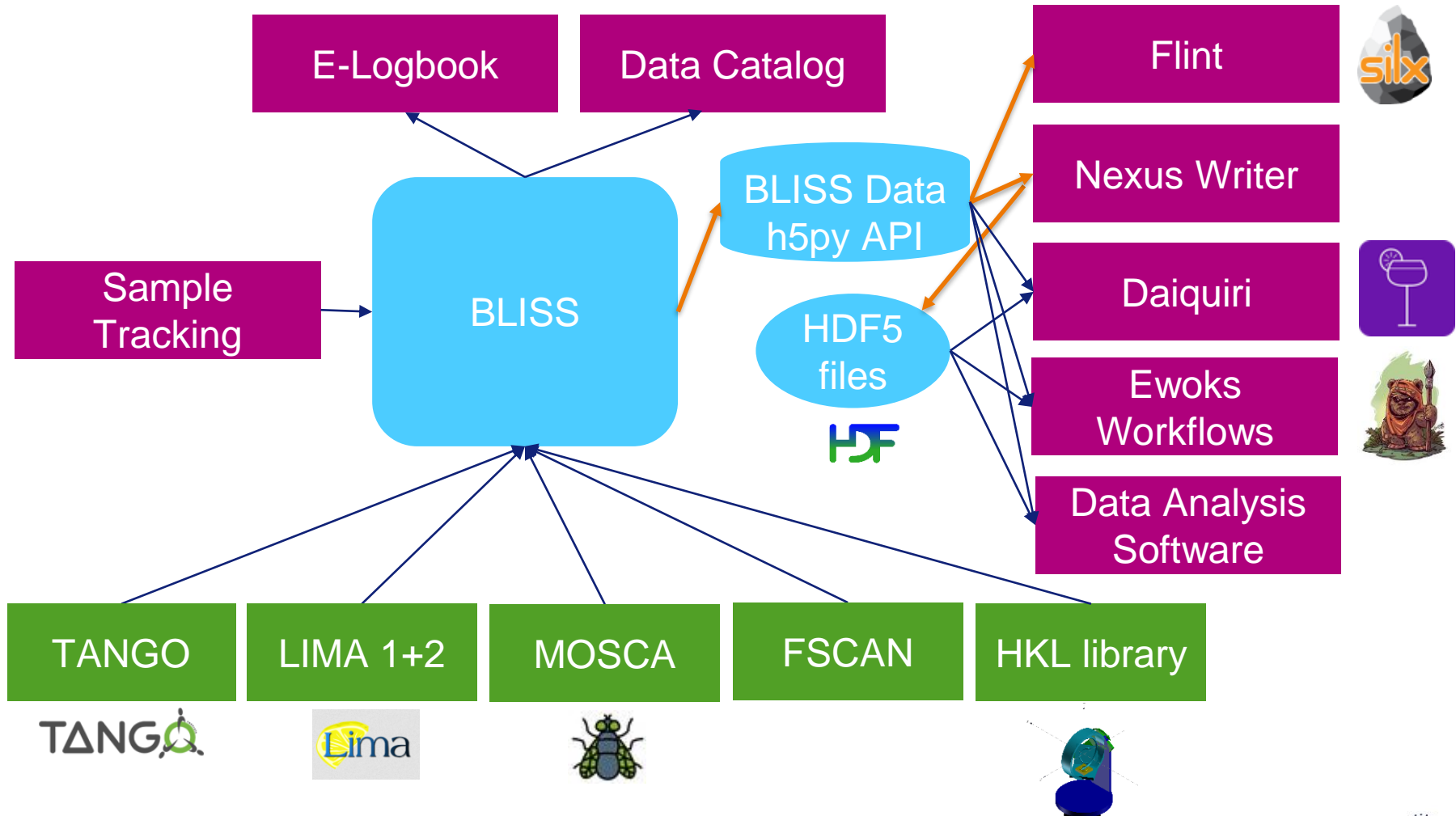
### BLISS Layer:

- BLISS: Experiment sequencing and data acquisition system, REDIS as in-memory storage
- BLISS Data: Interface library to stream acquired data from REDIS or from other in-memory data sources.
- Flint: Live data display of acquired data. Can display scan data or user data
- Nexus Writer: Saving of acquired data in a Nexus compatible HDF5 file tree for an experiment

### High Level Layer:

- EWOKS: On- and offline workflow system for data reduction and data analysis
- Daiquiri: Web framework for experiment GUIs

## Software Modules around BLISS



## Common interface for 2D image acquisition

- Starting, stopping, triggering, reading, saving

## Common interface for 2D image manipulation

- Binning, flipping, ROIs, ROI collections, dark and flat subtraction, etc

## 160 detectors running with LIMA at the ESRF

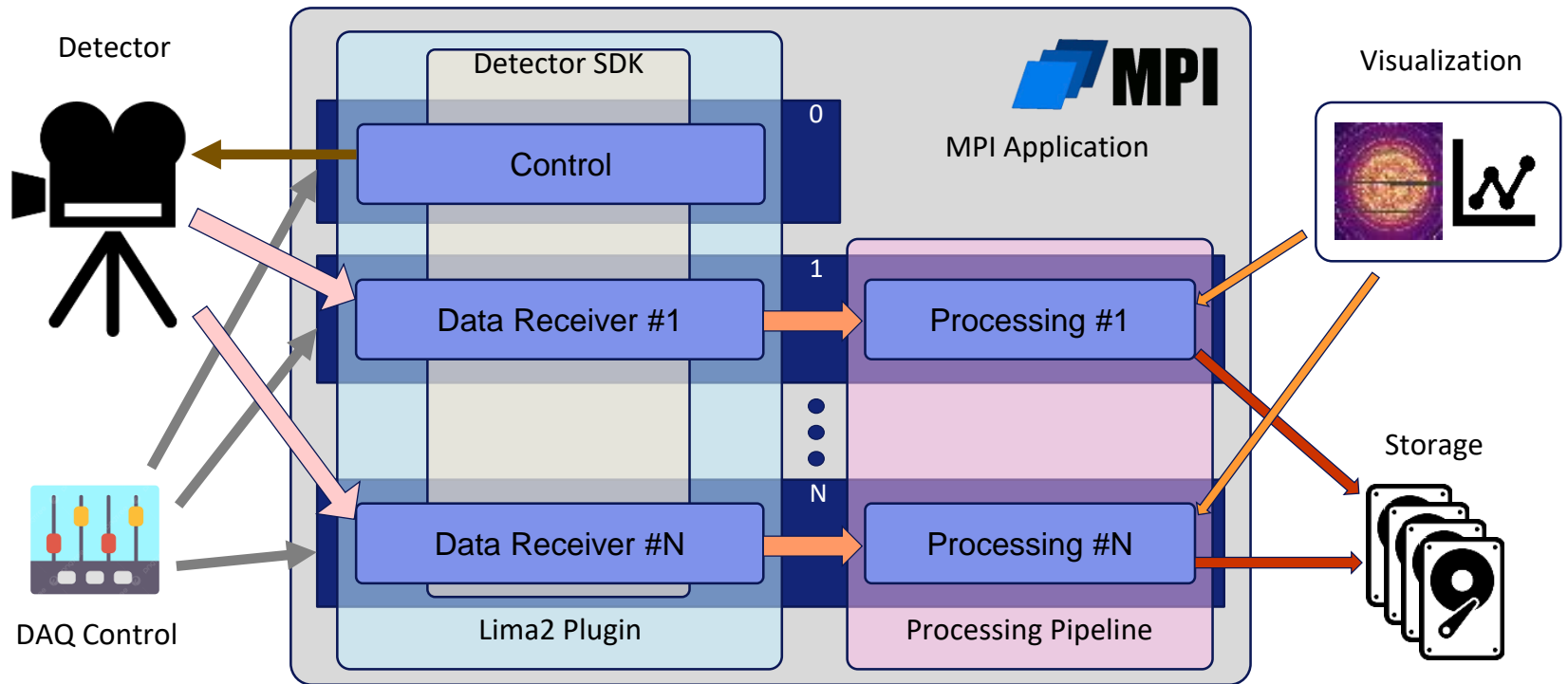
- 14 Frelon
- 17 Maxipix (Single chip, 2x2, 5x1, Meta 2x (3x1) )
- 15 Dectris Eiger2
- 10 Dectris Pilatus3
- 70 GigaE video camera: Basler, Prosilica, PointGrey, uEye
- 4 Andor I-Kon ccd, Zyla, Neo, Marana cmos
- 4 imXPAD
- 10 PCO Dimax & Edge, Edge HS, 2K, Camlink and USB
- 3 Perkin Elmer flat panel
- 2 Dexela flat panel
- 2 RoperScientific (aka Princeton)
- 3 Rayonix HS ccd
- 2 PSI Eiger 2M and 500K, 2 JungFrau 4M
- 1 FLI ccd
- 2 Advacam Minipix
- 2 Tucsen Dhyana cmos





Provide **scalable** data acquisition and **low latency** processing

Evolution of LIMA towards distributed systems



## Common interface for 1D data acquisition

- Starting, stopping, triggering, reading, saving

## Common interface for 1D data manipulation

- ROI, statistics

## Available detectors

- Mercury, FalconX, OceanOptics, Hamamatsu, XGLab

## Still under development

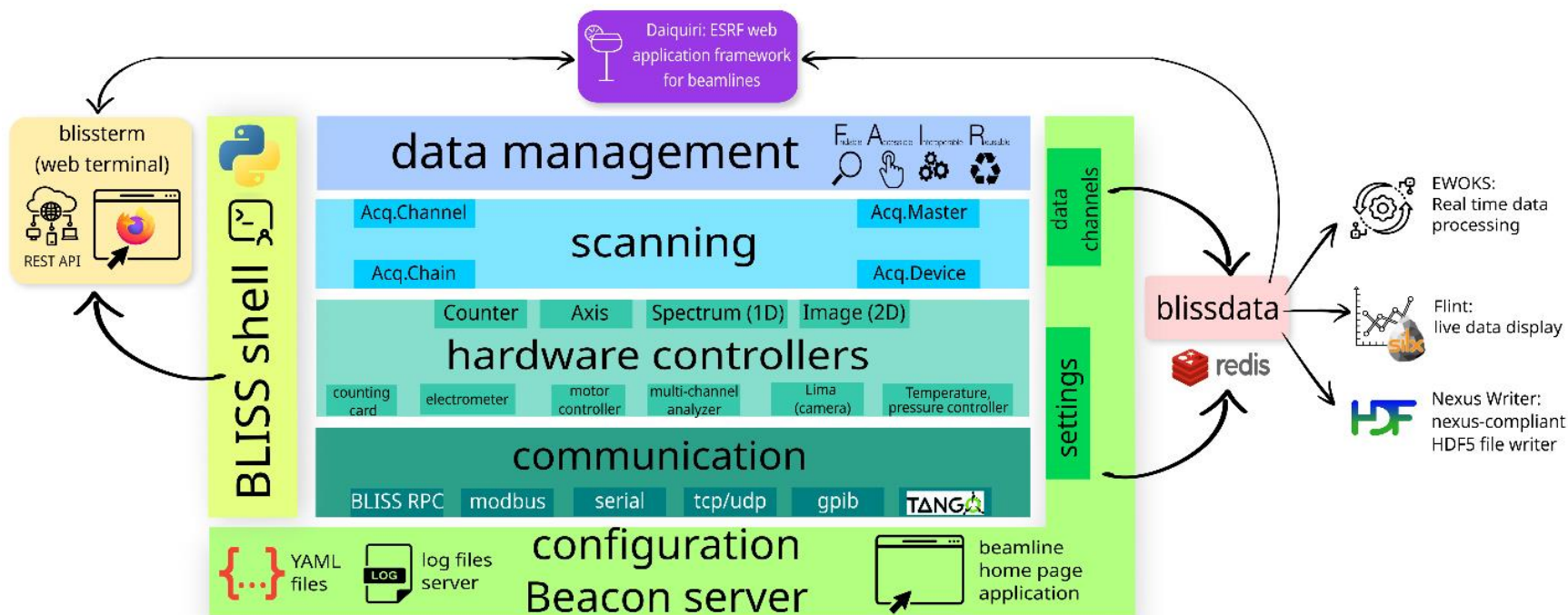
## Command line driven data acquisition sequencer written in Python

### Main concepts

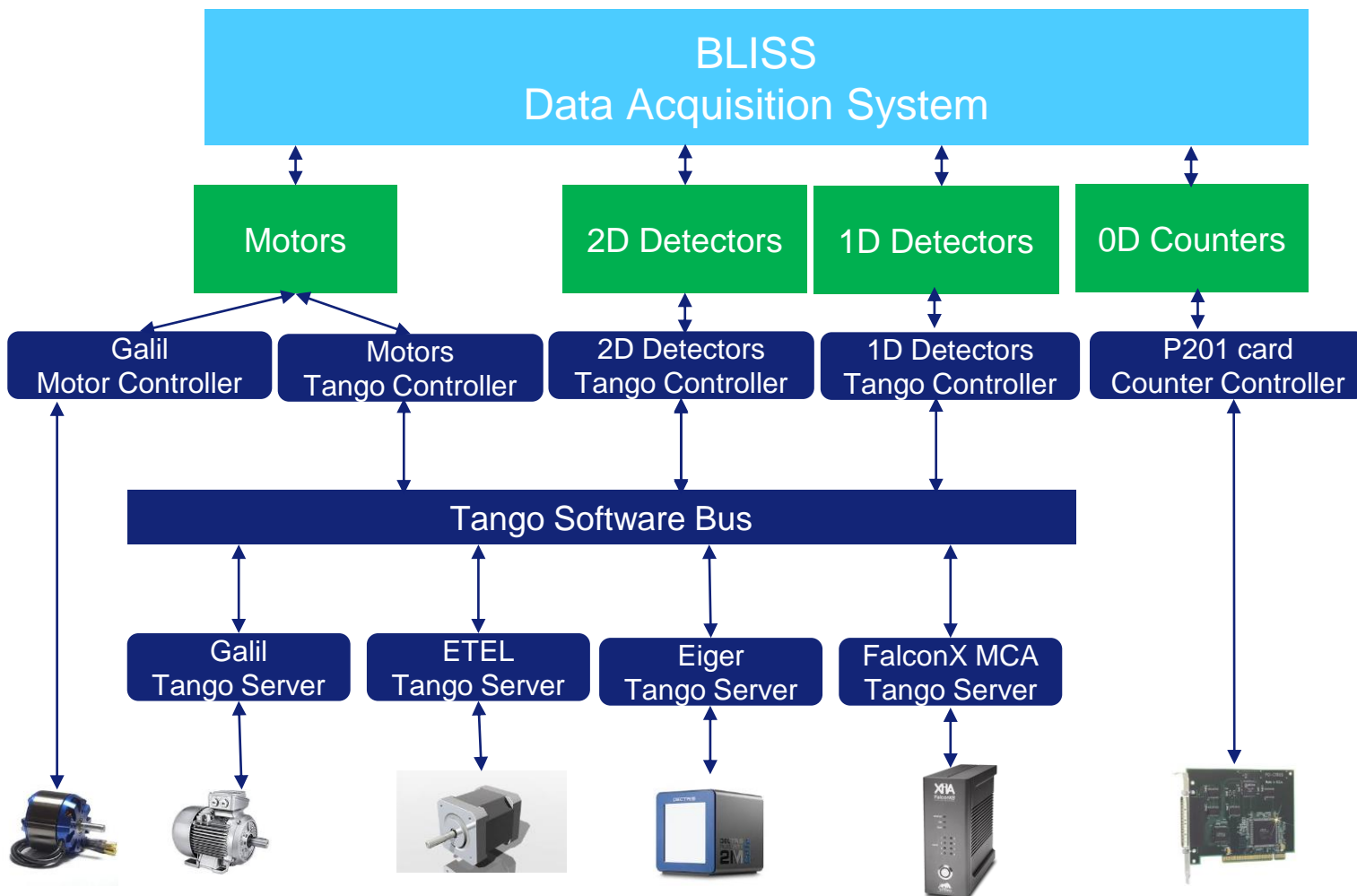
- **Hardware abstraction layer** for all instrumentation used during a data acquisition sequence  
*Motors, counters, monochromators, spectrometers, diffractometers, 2D detectors, etc.*
- **A generic scan engine** for step and continuous scans  
*The use of trajectories and HKL space is possible with all scans*
- **Decoupling of data acquisition** from data saving and analysis  
*All data buffered in memory. Allows higher acquisition speed without blocking*
- **Coherent HDF5 storage** of all acquired data at high speed and for large data volumes  
*All data of a proposal, its samples and the produced datasets is saved as a coherent HDF5 data tree*
- **Live data display** of all acquired data  
*Immediate visibility of acquisition results for the user*
- **Easy configuration** of hardware and experimental environment  
*Switch between predefined acquisitions set-ups on the fly*
- **PyTango** to interface any device from the Tango world  
*<https://www.tango-controls.org>*

<https://bliss.gitlab-pages.esrf.fr/bliss/master>

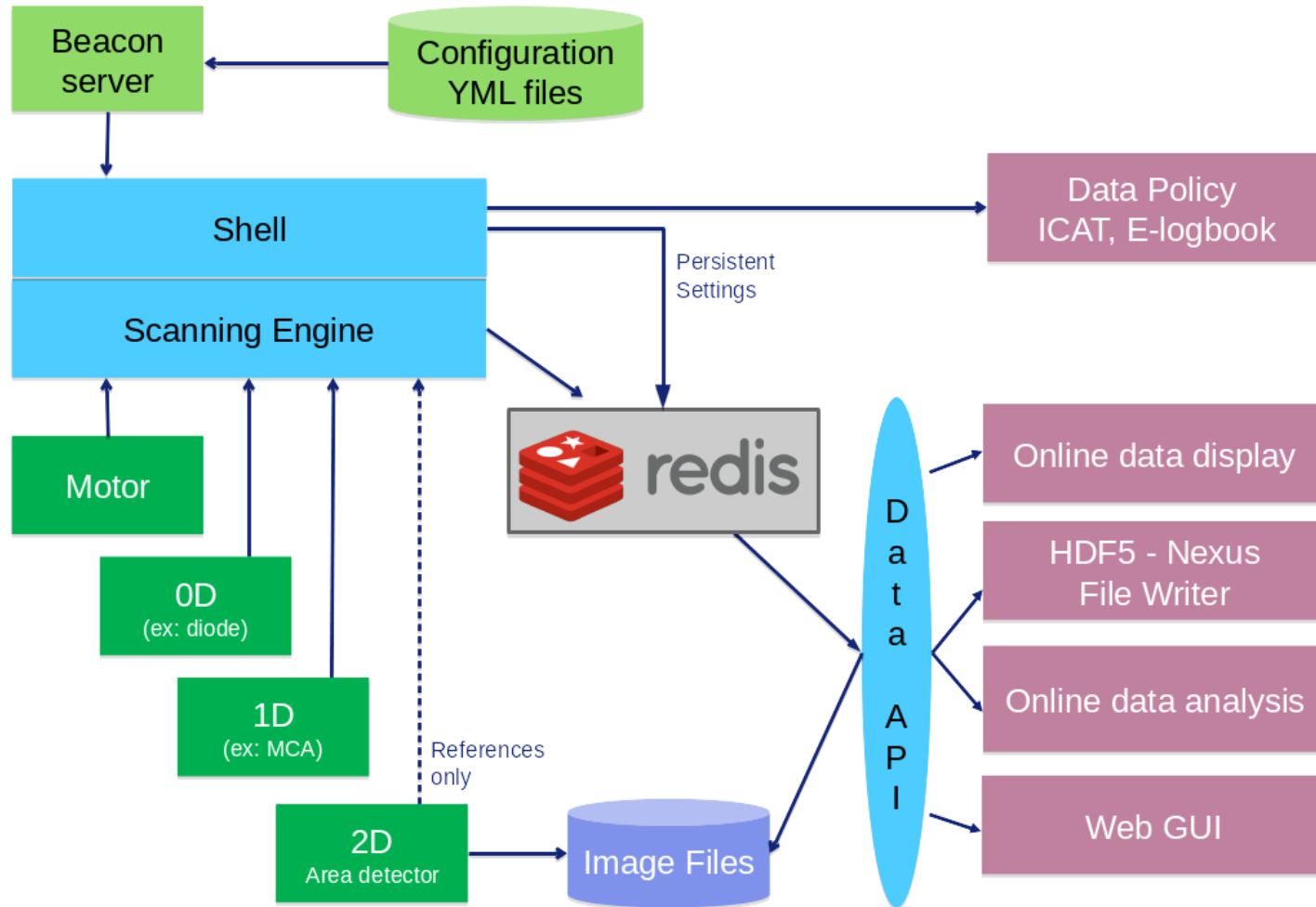
## Schematic view of the BLISS software layers



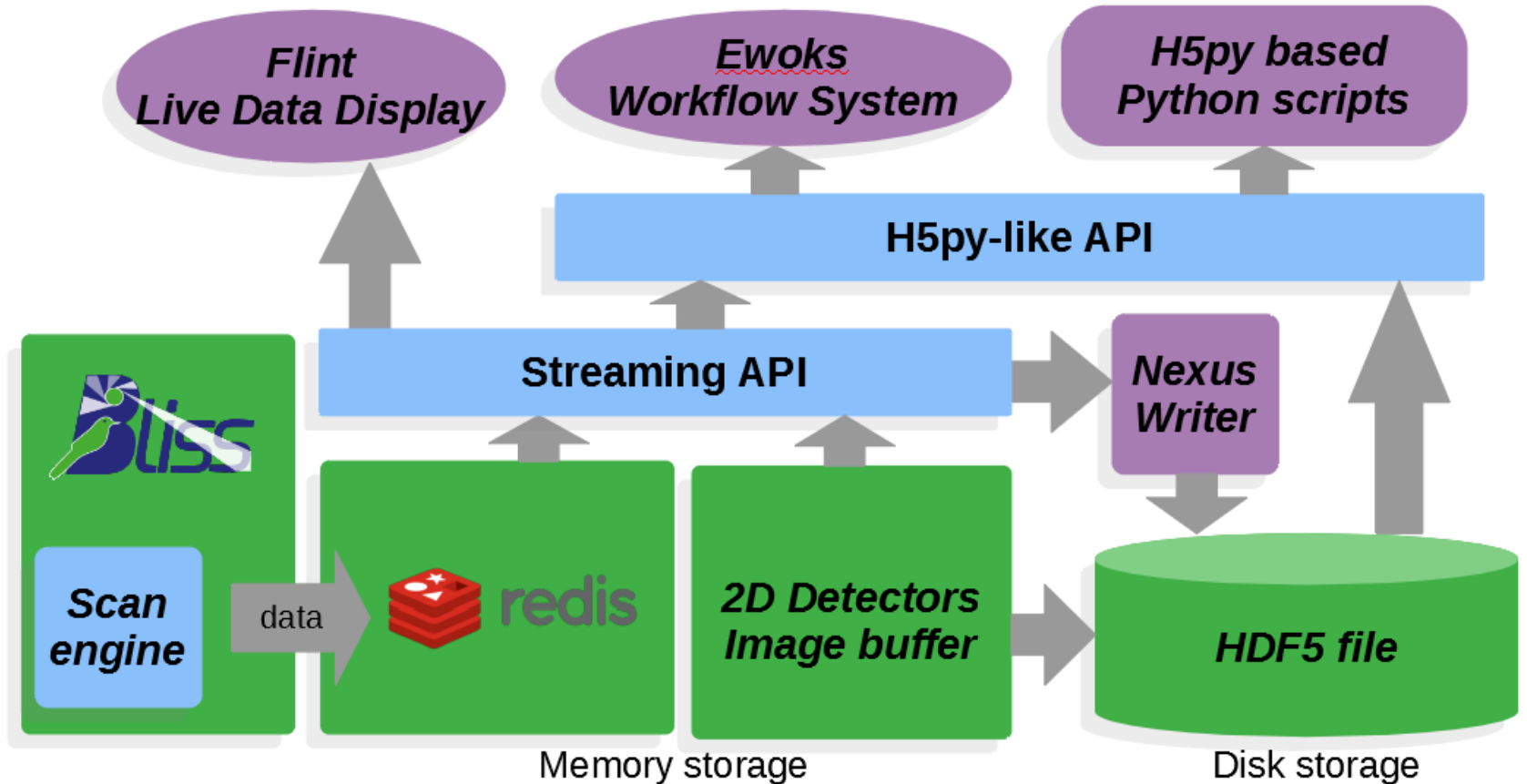
## Direct hardware access or underlying control system?



## Decoupling of data acquisition from data saving and analysis



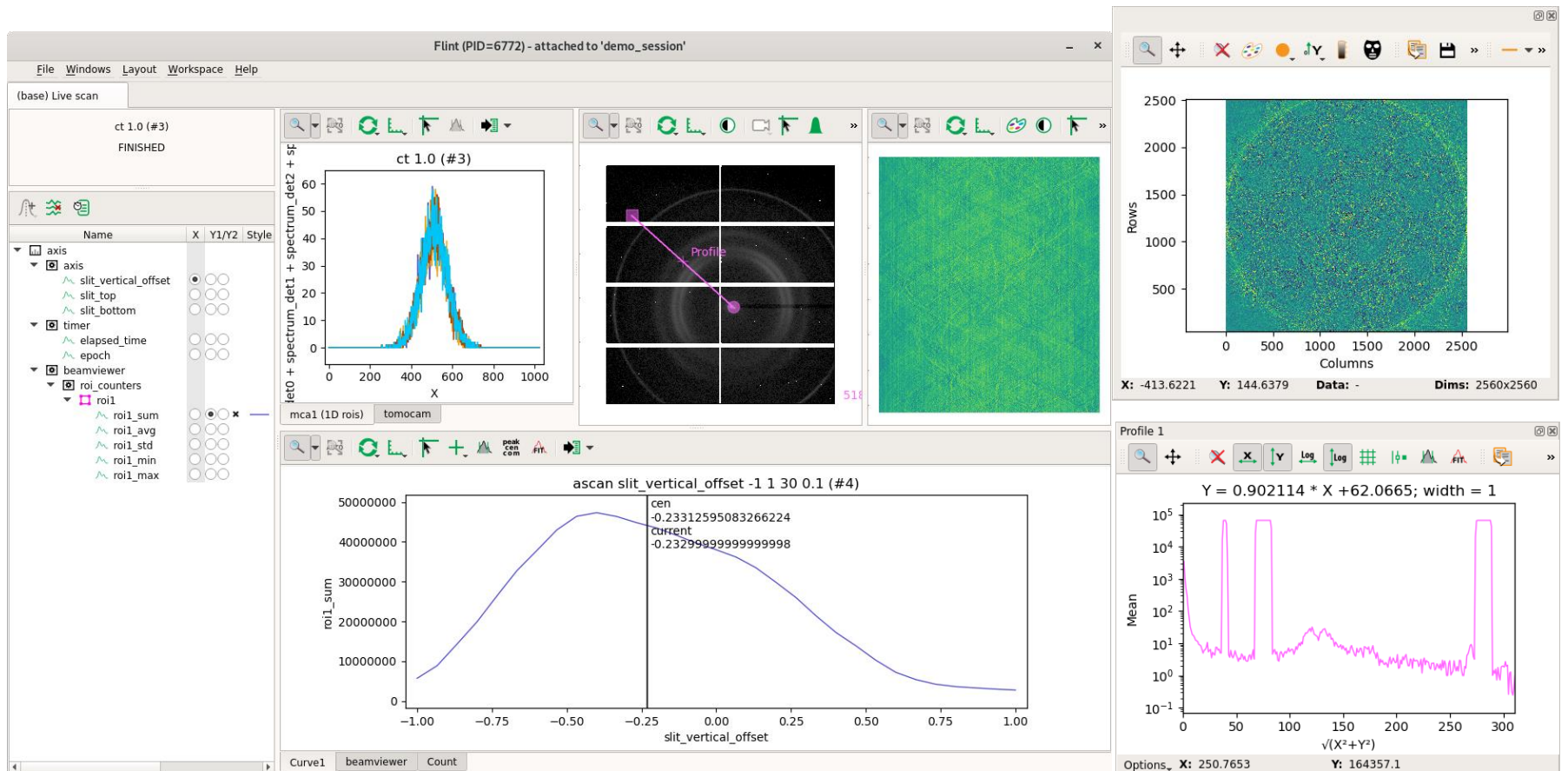
## Data streaming APIs



## Flint - Live data display

Live scan data

Calculated data can be pushed to Flint





## NEXUS Writer - Scan data and meta data saving

HDF5 files with Nexus tags

Coherent HDF5 file tree for all data sets of an experiment

The screenshot displays the Silx viewer interface with a file tree on the left and a data panel on the right. The file tree is organized as follows:

- ihls3397\_HA-900\_6.48um\_Antaeusuchus\_skeletalchron\_0001.h5
  - HA-900\_6.48um\_Antaeusuchus\_skeletalchron\_0001\_0001\_1.1
    - end\_time
    - instrument
    - measurement
    - scan\_numbers
    - sample
      - start\_time
      - technique
      - detector
      - optic
        - magnification
        - name
        - sample\_pixel\_size
        - scintillator
        - type
      - saving
        - beamline
        - frames\_per\_file
        - image\_file\_format
        - path
      - scan
        - comment
        - dark\_n
        - energy
        - exposure\_time
        - field\_of\_view
        - flat\_n
        - flat\_on
        - latency\_time
        - motor
          - name
          - nb\_scans
          - sample\_detector\_distance
          - scan\_range
          - scan\_type
          - sequence
          - source\_sample\_distance
          - start\_nb
          - tomo\_n
        - scan\_flags
        - subsans
        - title

The data panel on the right shows the following content:

```

Data
0 2
1 3
2 4
3 5
    
```

## Experiment GUI examples: Tomography

Daiquiri UI: bl Ring Current 4 Front End OPEN Energy 13 Hi,Test TU

**Scan status**

- Data collection: 7
- Scan: 680094776
- Status: **FINISHED**
- Progress: **Dark Flat Step scan Return**
- Description: Done

**Sample stage**

sr **READY**

**Sinogram**

Solid ▾

**Reconstructed slice**

Worker **DONE**

64

**Projection**

## Experiment GUI examples: XRF Mapping

Daiquiri UI: ID21

Ring Current: 195.12 | Front End: RUNNING | PSS Interlock: ON | Absorber 1: OPEN | Absorber 2: OPEN | HJd21 IO

Sum | Snap | Off | Mosaic | POI | ROI | LOI | Measure | Pan | Move | Clamp | Fill | Centre | Save | Canvas | Images

M8

#	Type	Size	Data	↑	↓	Q
1625	ROI	35x40 μm	Data	↑	↓	Q
1626	ROI	90x95 μm	Data	↑	↓	Q
1627	ROI	45x45 μm	Data	↑	↓	Q
1628	ROI		Data	↑	↓	Q
1629	ROI		Data	↑	↓	Q
1630	ROI		Data	↑	↓	Q
1631	ROI		Data	↑	↓	Q
1632	ROI		Data	↑	↓	Q
1633	ROI		Data	↑	↓	Q
1634	ROI		Data	↑	↓	Q
1635	ROI		Data	↑	↓	Q

Data Collections

Id	Start	Took	Status	Type
1512	09-10-2020 10:16:51	4 min	OK	XRF map

Maps

Id	DC	ROI	Px	Py	Visibility	Settings	Delete	
<input type="checkbox"/>	779	1512	S-Ka1	45	45	👁	⚙️	✖
<input type="checkbox"/>	780	1512	P-Ka1	45	45	👁	⚙️	✖
<input type="checkbox"/>	781	1512	Si-Ka1	45	45	👁	⚙️	✖

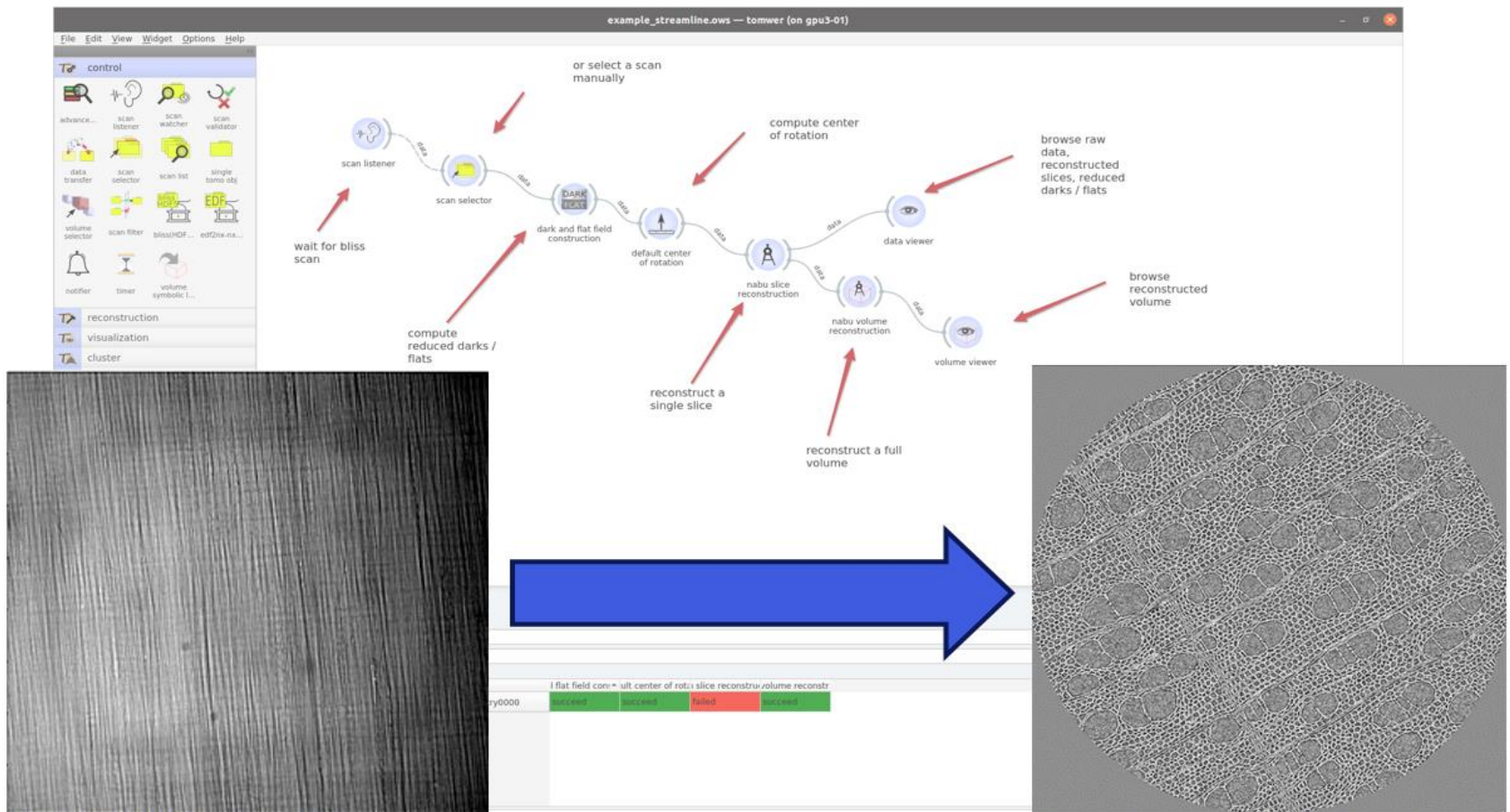
Id	Red	ROI	Green	ROI	Blue	ROI
No composite maps for this object						

samy READY | samz READY | sampy READY | sampz READY | zoom\_MP READY | samx READY | vim ACQUIRING | wcid21d ON | sample\_stage\_MP READY

6.3005 | 0.1 | 27.0436 | 0.1 | 58.93 | 5 | 15.8731 | 5 | x12 | Move | 0.3497 | 0.01 | 0.01 | Live | Backlight | 0 | unknown | Move

## Workflow for Tomography reconstruction

Tomography reconstruction (ID19, BM05, BM18, ID11, ID16B)



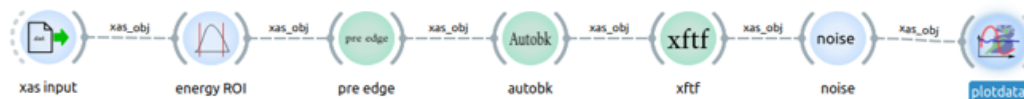
**Inputs:** BLISS scan data  
(darks, flats, projections + metadata)

**Outputs:** reconstructed volumes



## Workflow for EXAFS visualization

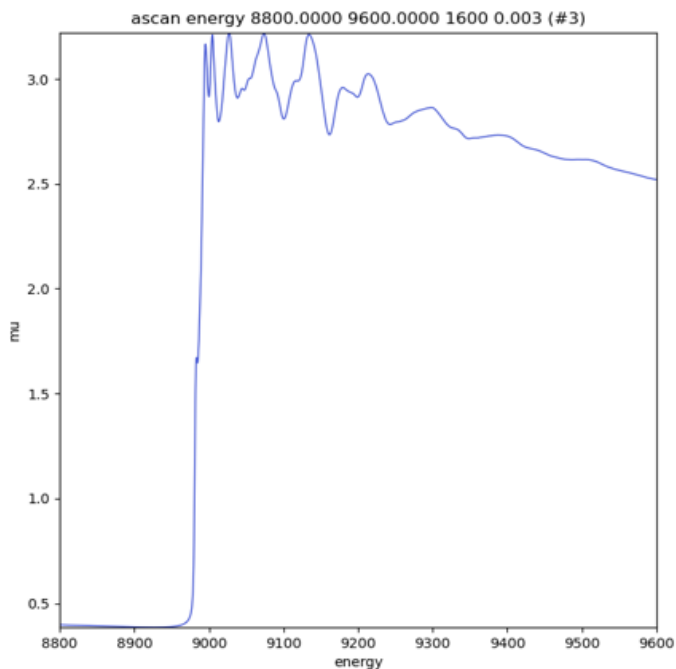
EXAFS visualization (BM23)



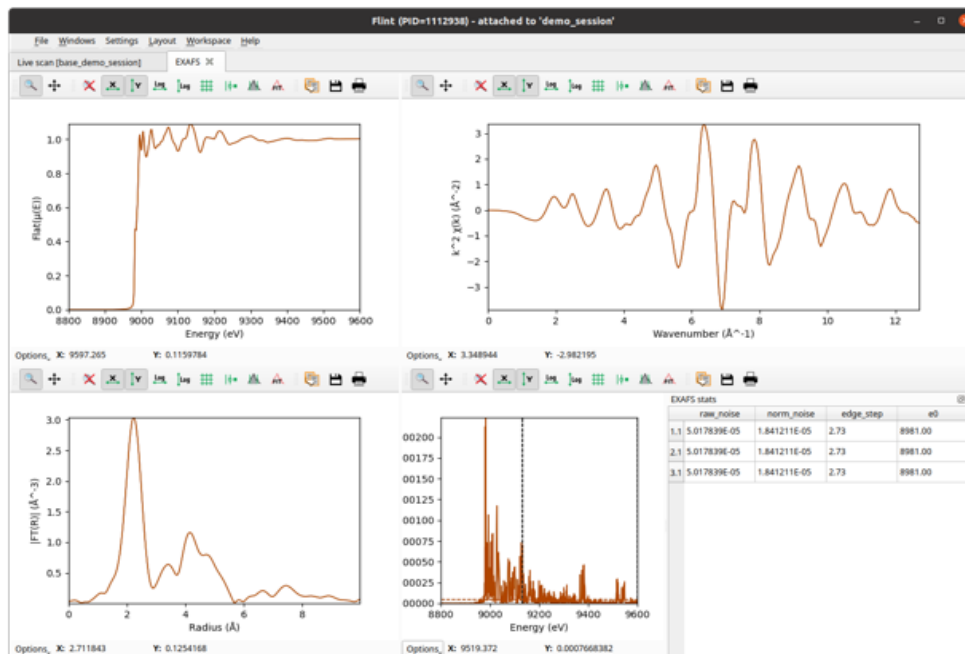
Data acquisition



On-line EXAFS visualization



EXAFS spectrum



Parameter space in which scientific decisions are made

### Collaboration is possible on all the different software modules!

Tango, LIMA and the HKL library are already collaborative projects

Data Portal and E-logbooks have been presented to other institutes

BLISS Data API with Flint and NexusWriter

- Prototype version at ALBA connected to Sardana
- Prototype version at DESY connected to Bluesky
- Prototype version at SLS connected to BEC

EWOKS is a meta workflow system that uses other workflow systems for automating experiments and data processing adapted to the use case.

DAIQUIRI

- Completely independent from controls system and scan engine
- Proof of concepts at SLS connected to BEC, DESY connected to Bluesky
- daiquiri-lib for shared UI components without committing to a full framework

### **BLISS and EWOKS in daily operation on 35 beamlines**

Abstraction for scanning (step or fly)

The use of trajectories and HKL space is possible with all scans

Live data display for all acquired data

Standardized HDF5/Nexus file tree for all data acquisition

In memory data buffers for on-line data analysis

Standardized data extraction API for on- and off-line data

On-line data processing at detector level (LIMA) or with workflows

Web GUIs for scientific applications



## Acknowledgements to

- The members of the software group for the development of all the different software tools
- Any Questions?