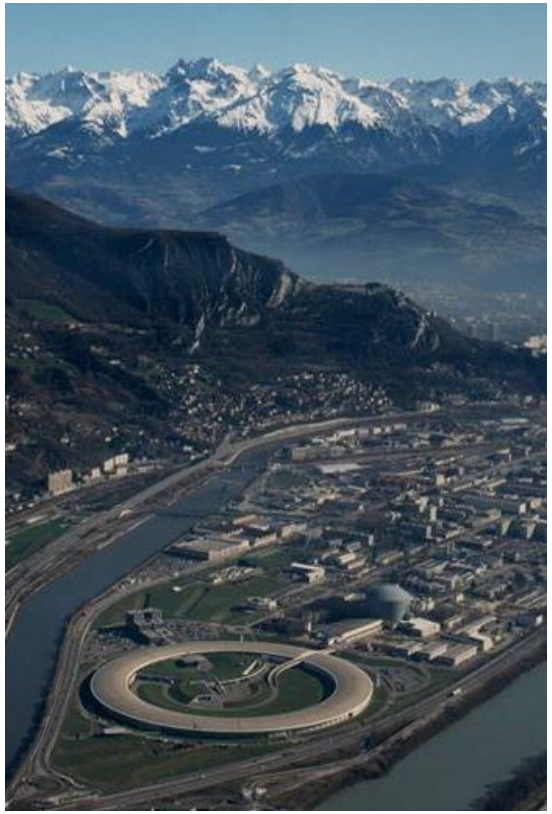

ESRF
The European Synchrotron

BLISS
BEAMLINE CONTROL AND DATA ACQUISITION



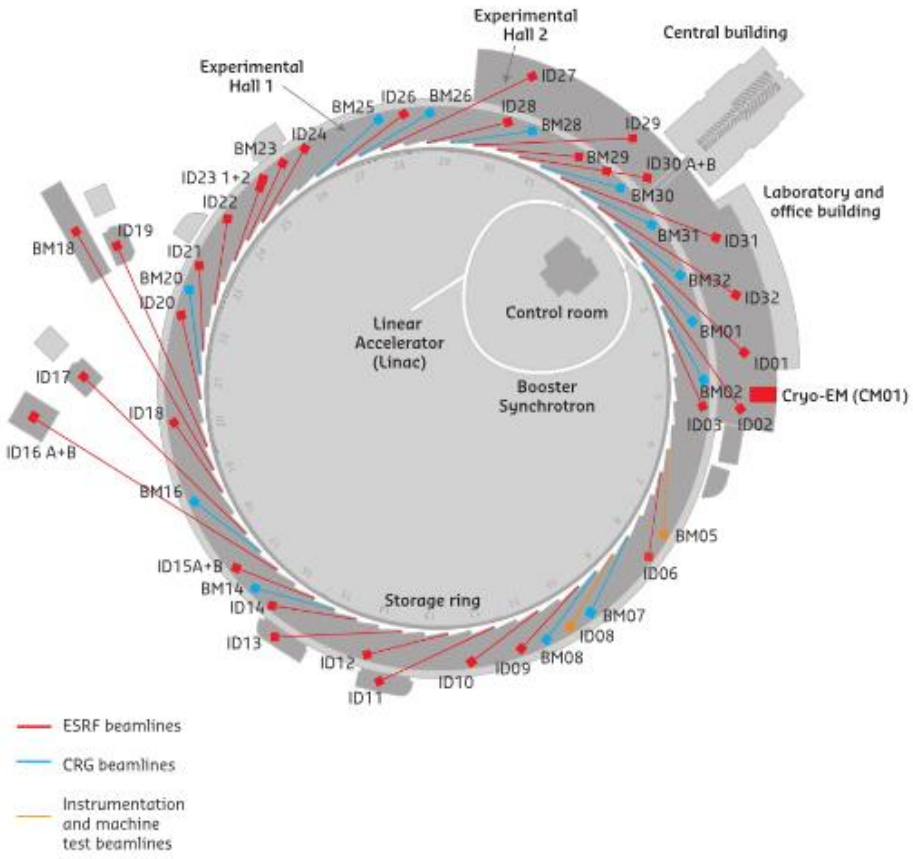
Outline

- Instrument Control
- Data Acquisition
- Data Access
- FAIR Data
- Conclusion

Jens Meyer on behalf of the ESRF Software Group

ESRF BEAMLINES AND EXPERIMENT TYPES

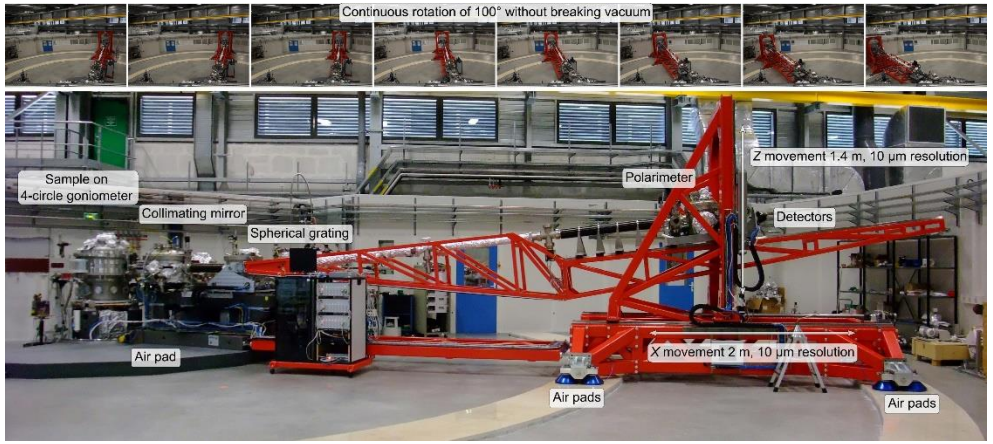
33 ESRF beamlines and 13 CRG beamlines

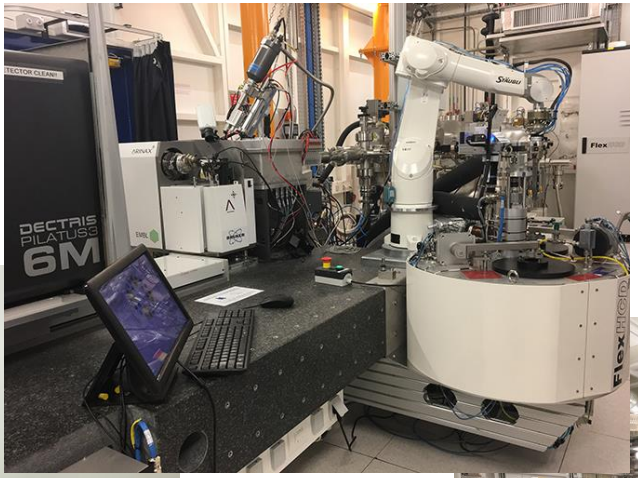


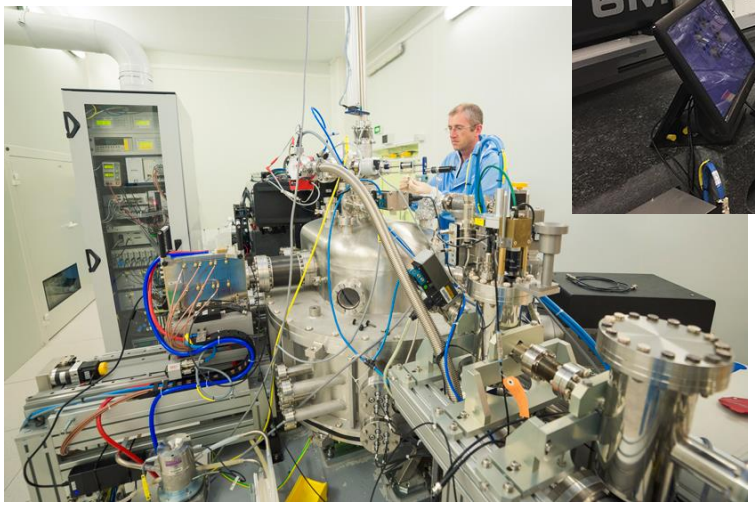
SOURCE POSITION	INDEPENDENT END-STATIONS	FIELD OF RESEARCH	STATUS	DATE
ID01	1	Microdiffraction imaging	Operational	Since 12/14
ID02	1	Time-resolved ultrasmall-angle X-ray scattering	Operational	Since 07/14
ID03	1	Hard X-ray diffraction microscopy	Construction	
ID06	1	Large volume press /Hard X-ray diffraction microscopy	Operational	Since 10/13
ID09	1	Time-resolved structural dynamics	Operational	Since 09/94
ID10	1	Soft interfaces and coherent scattering	Operational	Since 06/12
ID11	1	Materials science	Operational	Since 09/94
ID12	1	Polarisation-dependent X-ray spectroscopy	Operational	Since 01/95
ID13	1	Microfocus	Operational	Since 09/94
ID14	1	Nuclear scattering	Construction	
ID15A	0.85	Materials chemistry and engineering	Operational	Since 11/16
ID15B	0.5	High-pressure diffraction	Operational	Since 11/16
ID16A	1	Nano-imaging	Operational	Since 05/14
ID16B	1	Nano-analysis	Operational	Since 04/14
ID17	1	Medical	Operational	Since 05/97
ID18	1	Nuclear scattering	Operational	Since 01/96
ID19	1	Microtomography	Operational	Since 06/96
ID20	1	Inelastic X-ray scattering	Operational	Since 06/13
ID21	1	X-ray microscopy / IR spectroscopy	Operational	Since 12/97
ID22	1	High resolution powder diffraction	Operational	Since 05/14
ID23	2	Macromolecular crystallography MAD	Operational	Since 06/04
		Macromolecular crystallography microfocus	Operational	Since 09/05
ID24	0.5	Dispersive EXAFS	Operational	Since 12/21
ID26	1	X-ray absorption and emission	Operational	Since 11/97
ID27	1	High pressure	Operational	Since 11/21
ID28	1	X-ray scattering II	Operational	Since 12/98
ID29	1	Multiwavelength anomalous diffraction	Closed	Since 08/20
ID30A	2	Macromolecular crystallography	Operational	Since 07/14
ID30B	1	Macromolecular crystallography	Operational	Since 04/15
ID31	1	Interfaces and materials processing	Operational	Since 11/15
ID32	1	Soft X-ray spectroscopy	Operational	Since 11/14
BM18	1	Hierarchical tomography	Construction	Since 12/14
BM23	1	X-ray absorption spectroscopy	Operational	Since 01/21
BM29	1	Bio SAXS	Operational	Since 06/12
CM01	1	Cryo-EM	Operational	Since 11/17

46 Beamlines
More than 100 scientific techniques

ESRF EXPERIMENTAL SETUPS







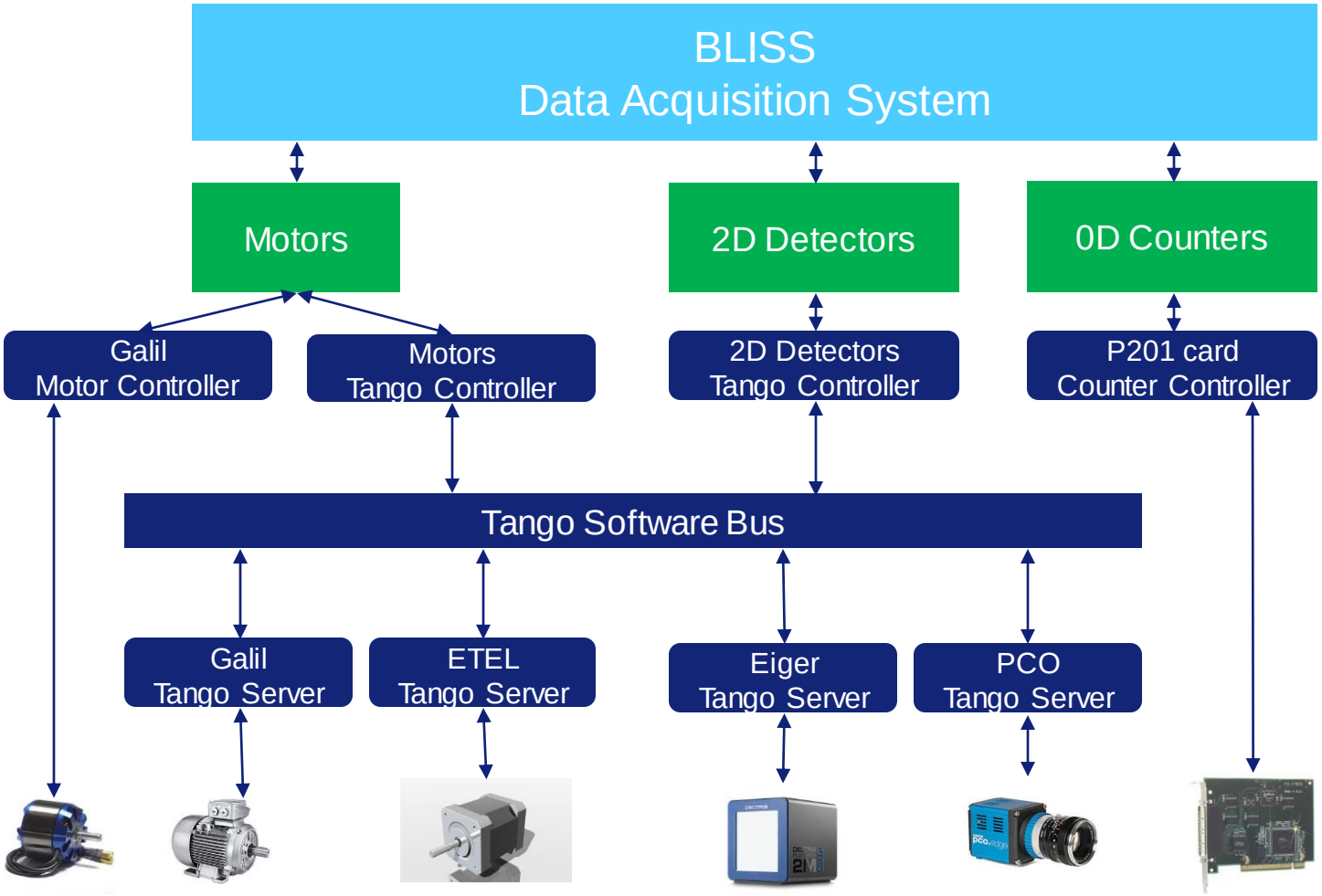
Command line driven data acquisition sequencer written in Python

Main concepts

- **Hardware abstraction layer** for all instrumentation used during a data acquisition sequence
  Motors, counters, monochromators, spectrometers, diffractometers, 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

Direct hardware access or underlying control system?



BLISS Hardware Abstraction Frameworks

Monochromators

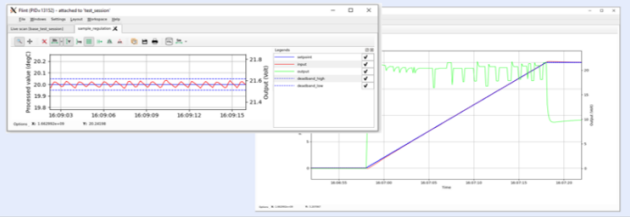
- Generic API
- Crystal manager
- Multi-layers compatibility
- Energy calculation
- Tracker motors (undulator, sample)
- Continuous scans and trajectories

Regulation

- Generic API
- Integrated hardware
- Custom regulation
- Monitoring/plotting with Flint
- Axis like control
- Tango Server

Monitoring and real-time plotting

Monitor the regulation in live through Flint, the BLISS data online visualization tool.
Follow the evolution of the process value, setpoint and ouput power over an adjustable time-window.



Spectrometers

- Generic API
- 3D positioners (Analyzers + Detector)
- Mixed crystals compatibility
- 2D detector compatibility
- 3D live monitoring plot (ray-tracing)
- Customizable geometries

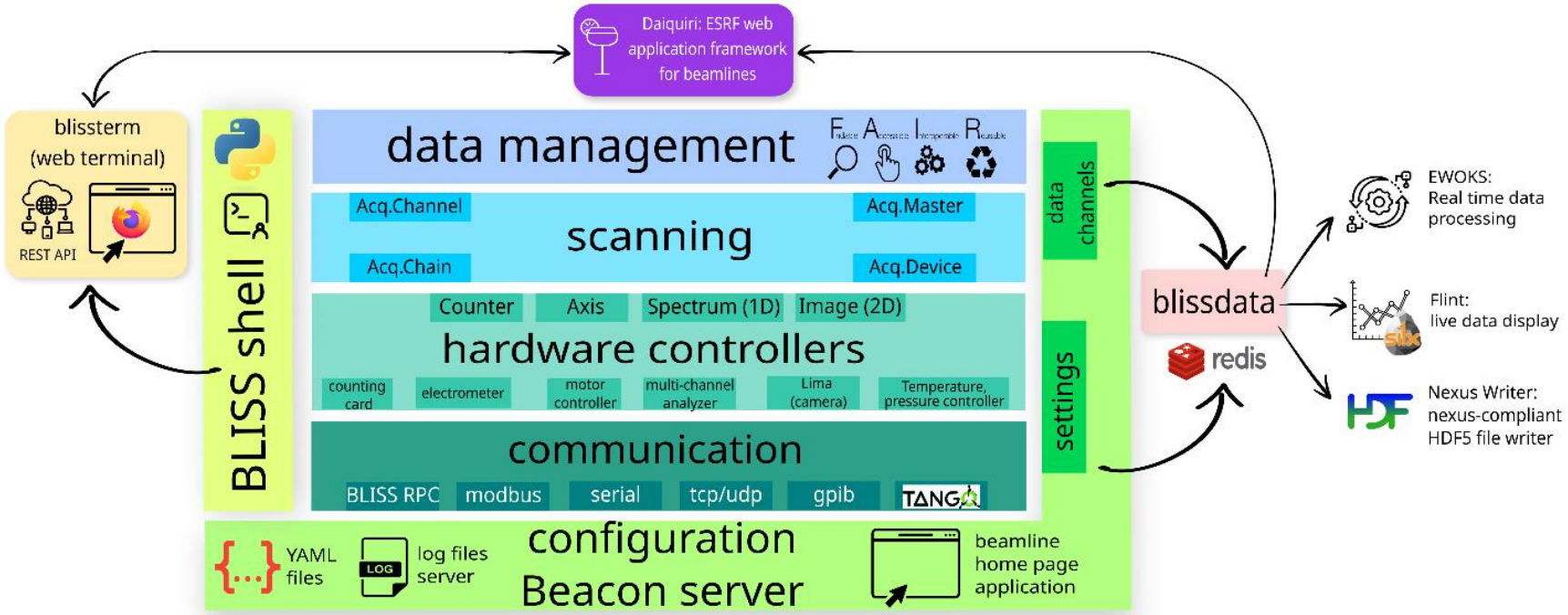
Diffractometers

- Generic API
- Based on Picca's HKL library
- 18 available geometries
- Different engines per geometry
- HKL scans and trajectories
- SPEC like commands

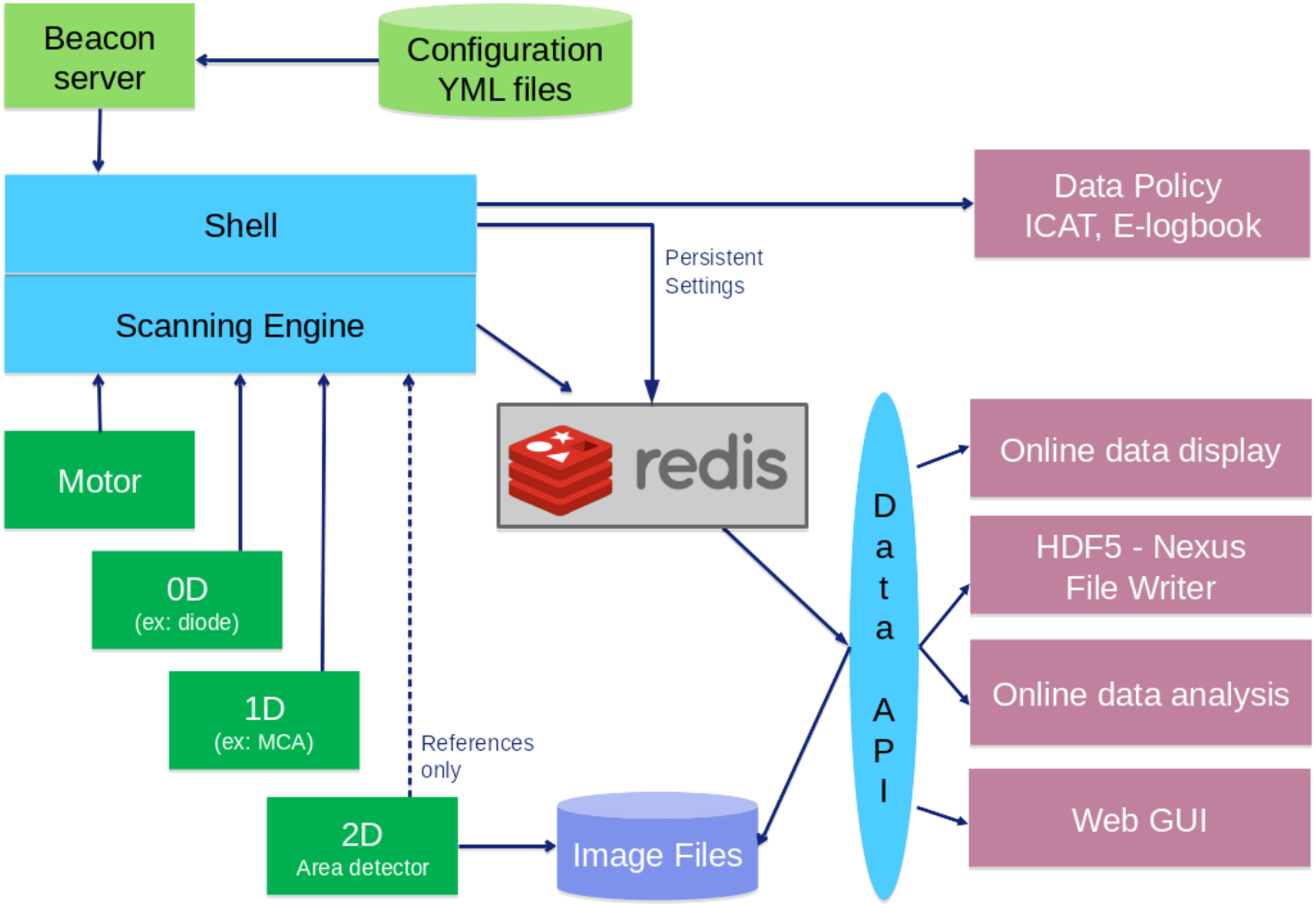
Easy declaration with YAML configuration file

```yaml
diffractometers:

  - name: d4ch
    module: diffractometers.diff_fourc
    class: DiffE4CH
    geometry: E4CH

    axes:
      - name: $roby
        tags: real omega
      - name: $robu
        tags: real chi
      - name: $robz
        tags: real phi
      - name: $robz2
        tags: real tth
      - name: $mono
        tags: real energy

      - name: H
        tags: hkl_h
      - name: K
        tags: hkl_k
      - name: L
        tags: hkl_l
      - name: Q
        tags: q_q
```

Schematic view of the BLISS software layers

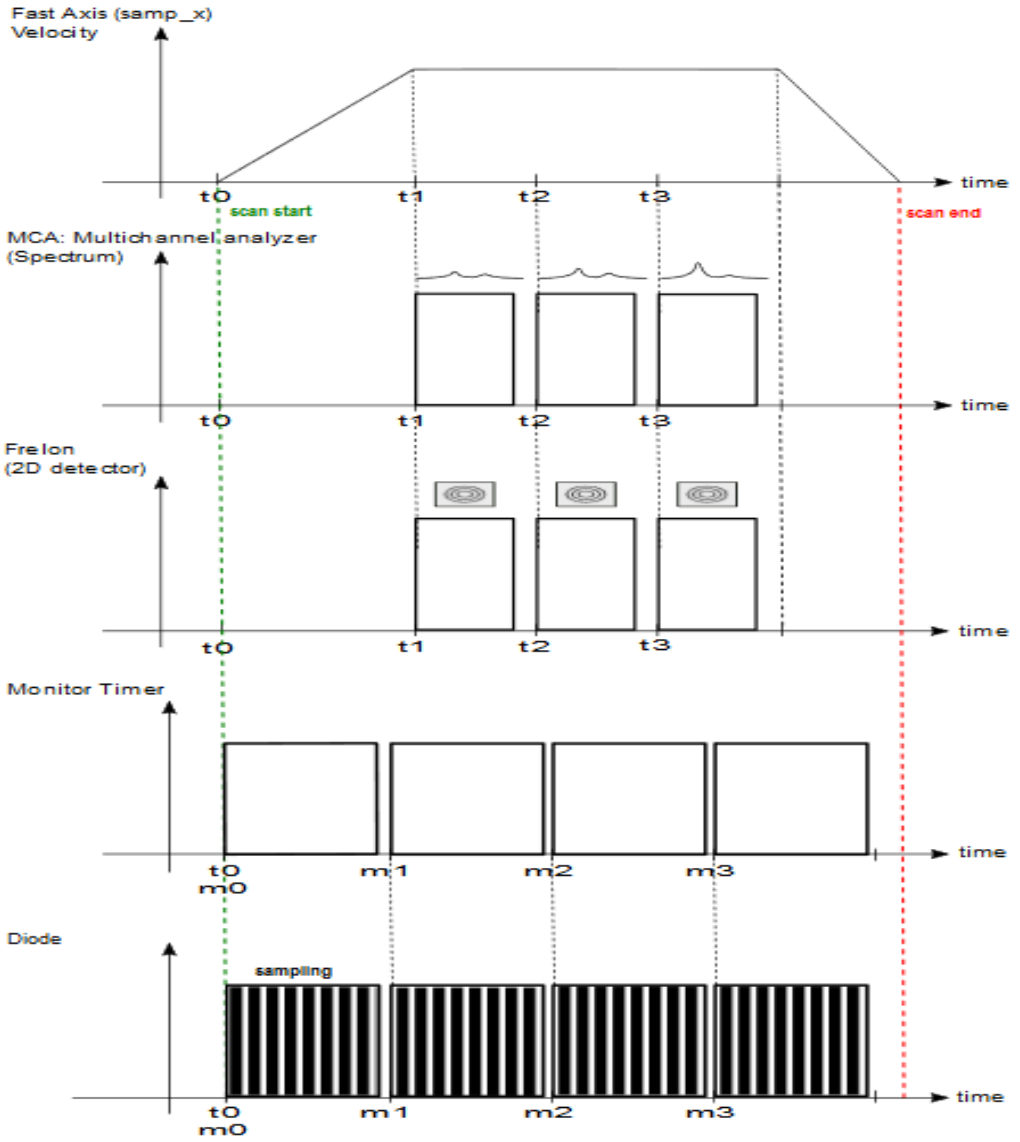


Decoupling of data acquisition from data saving and analysis



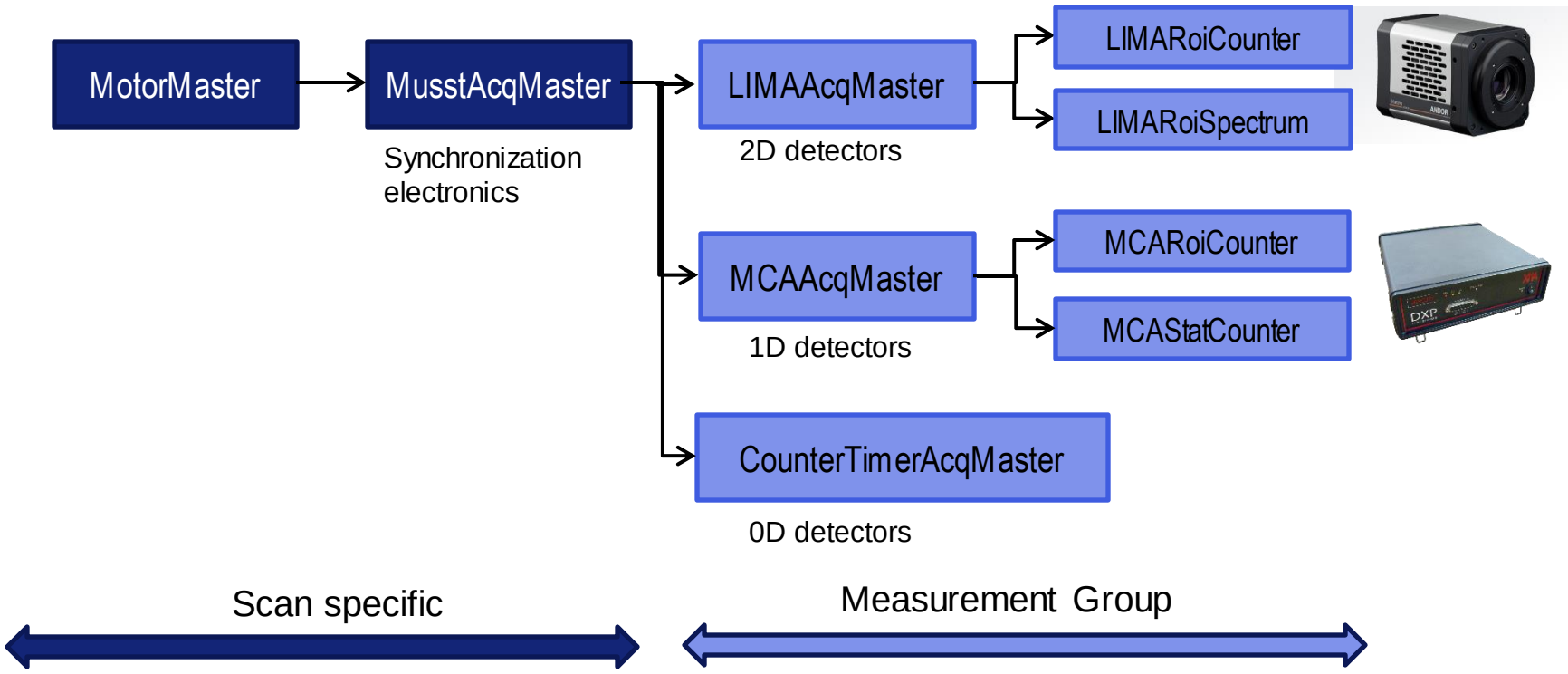
BUILDING A CONTINUOUS SCAN

- Motor:samp_x
  - MCA
    - spectrum
  - Lima
    - image
- Timer
  - Keithley
    - scalar



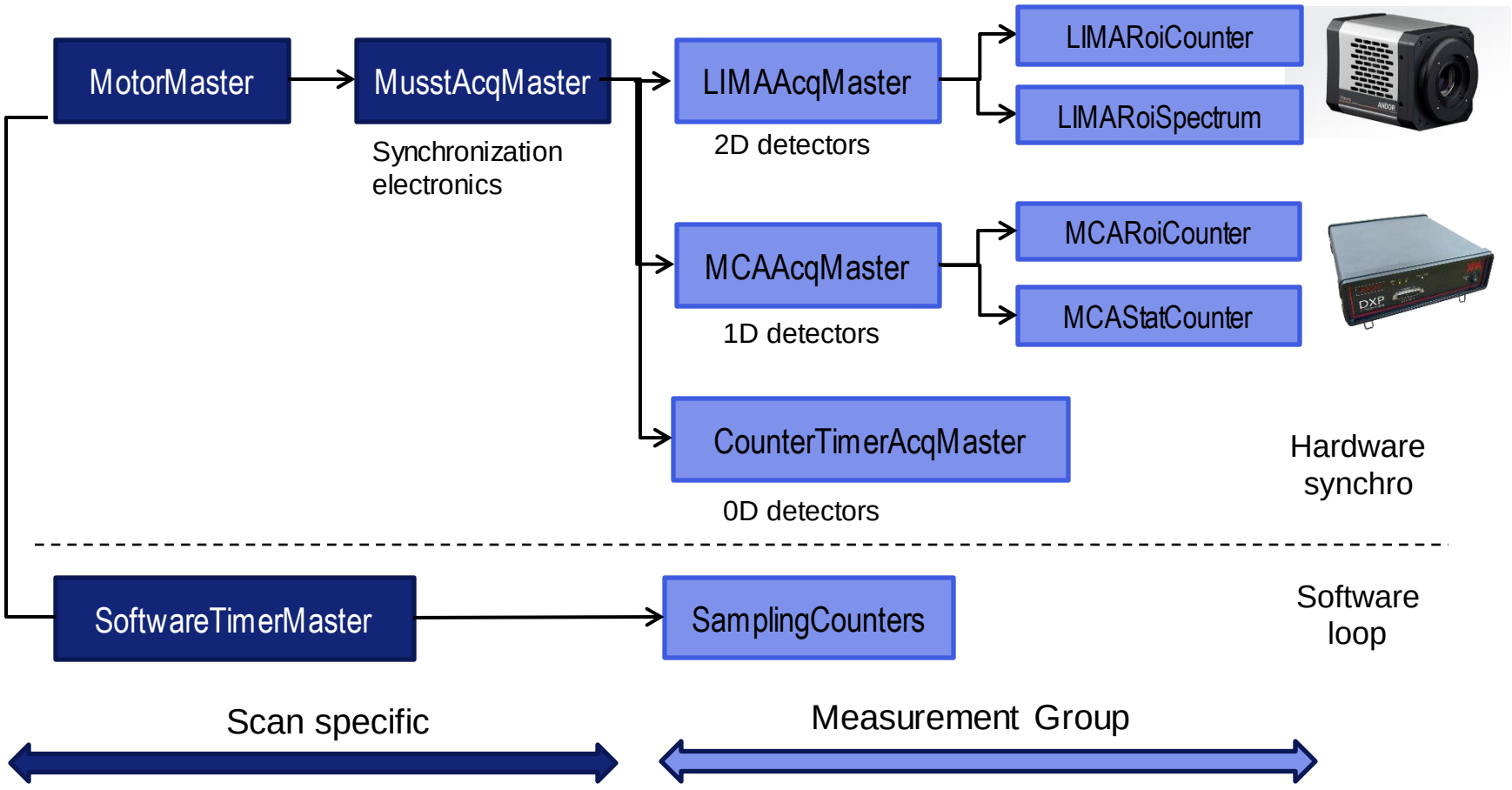
Writing a scan is writing an AcquisitionChain

AcquisitionChain is a tree of **AcquisitionObjects** with master/slave relations



SoftwareAcquisitionMaster : For counters that cannot be synchronized

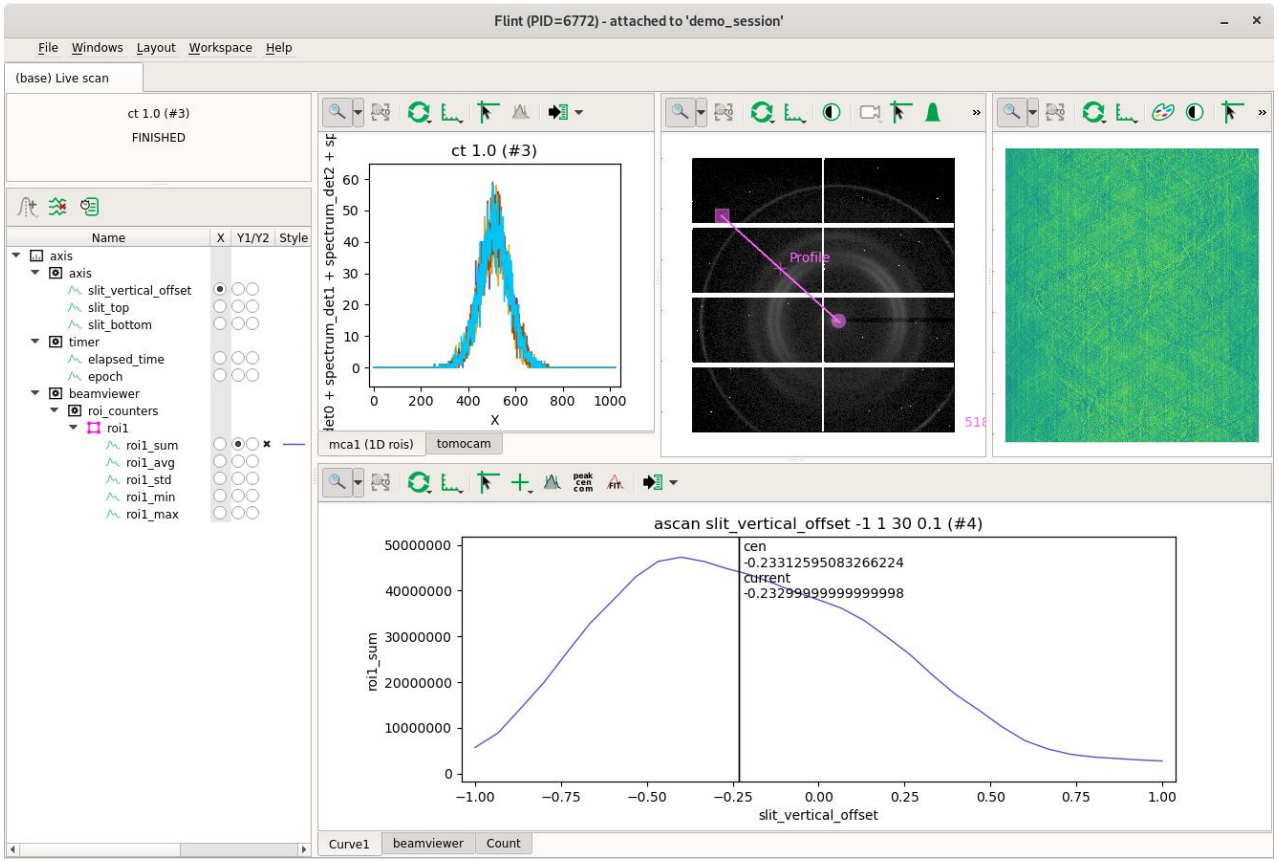
- Epoch counter provided to link the acquisition of the 2 masters

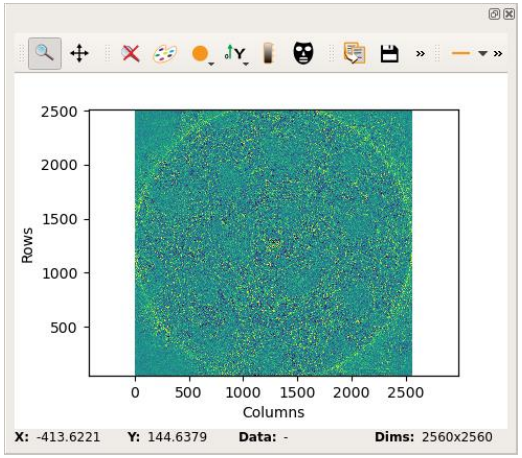


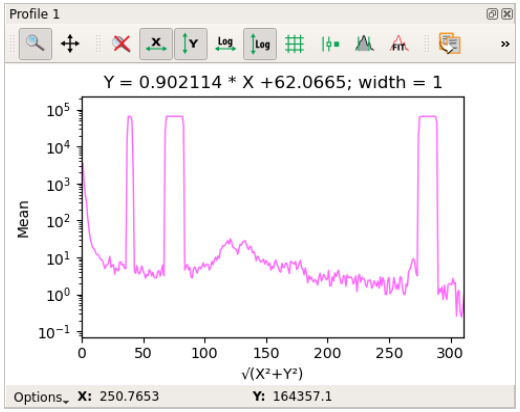
Flint - Live Data Display

Live scan data

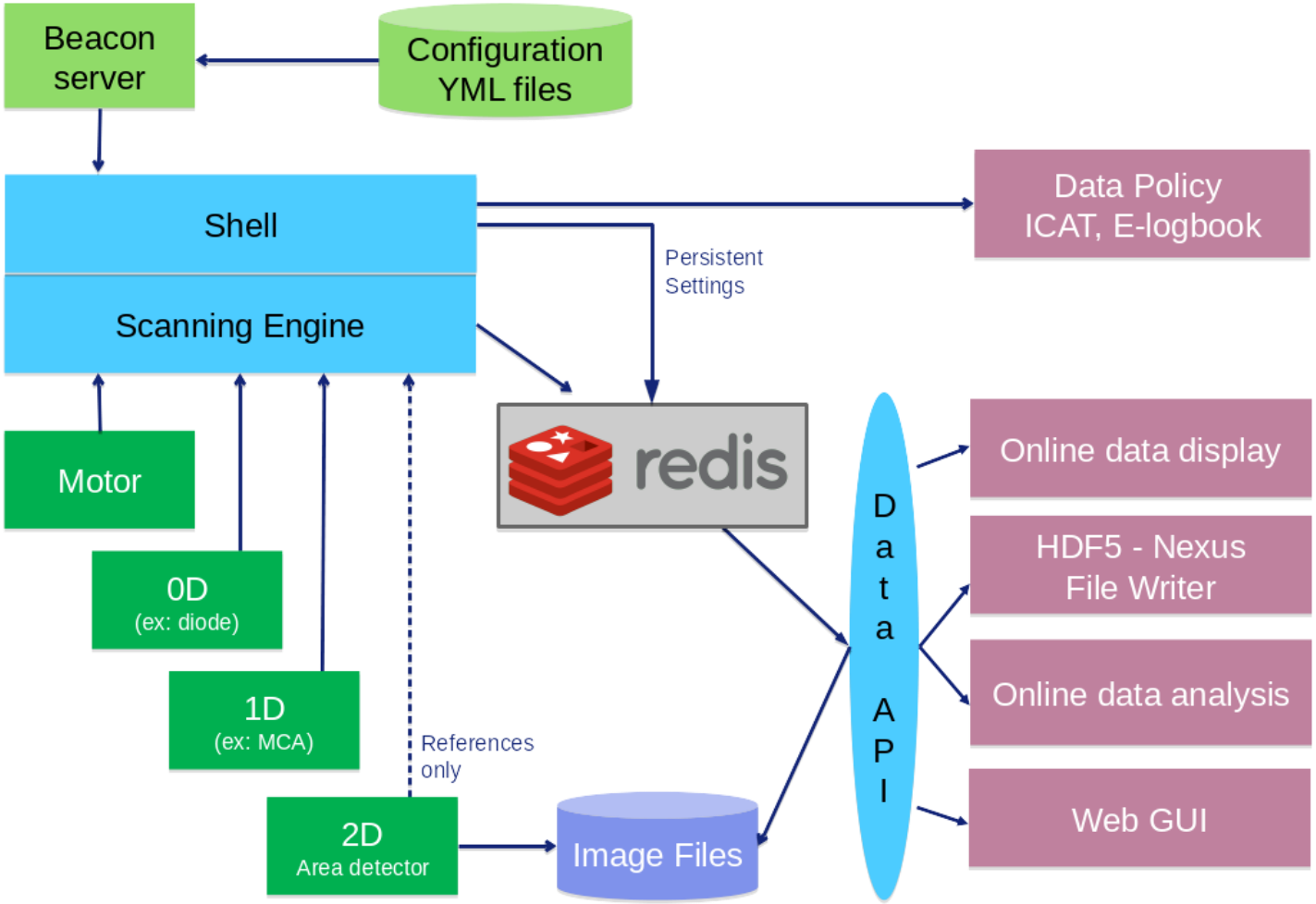
Calculated data can be pushed to Flint







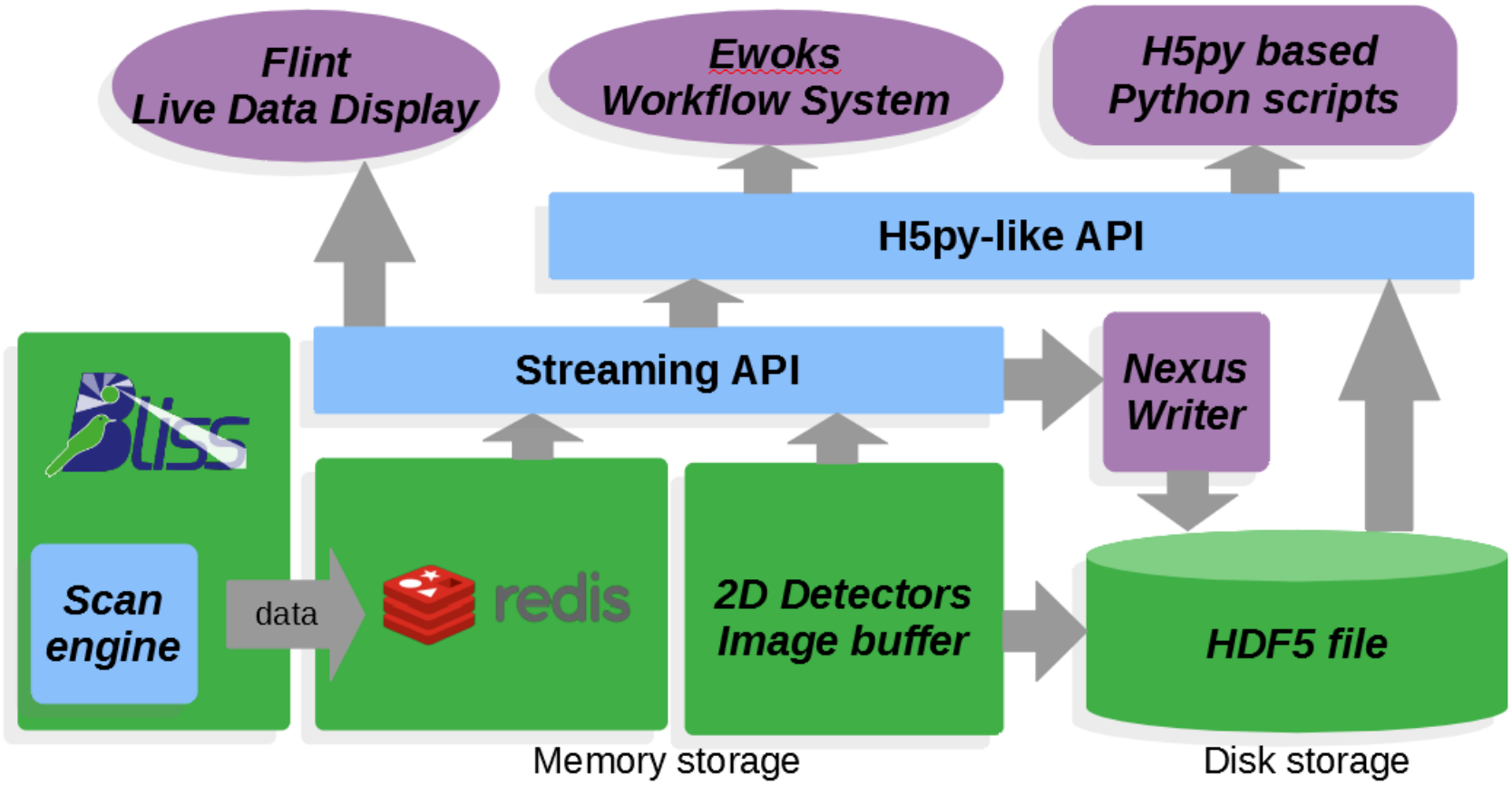
Decoupling of data acquisition from data saving and analysis



Streaming API

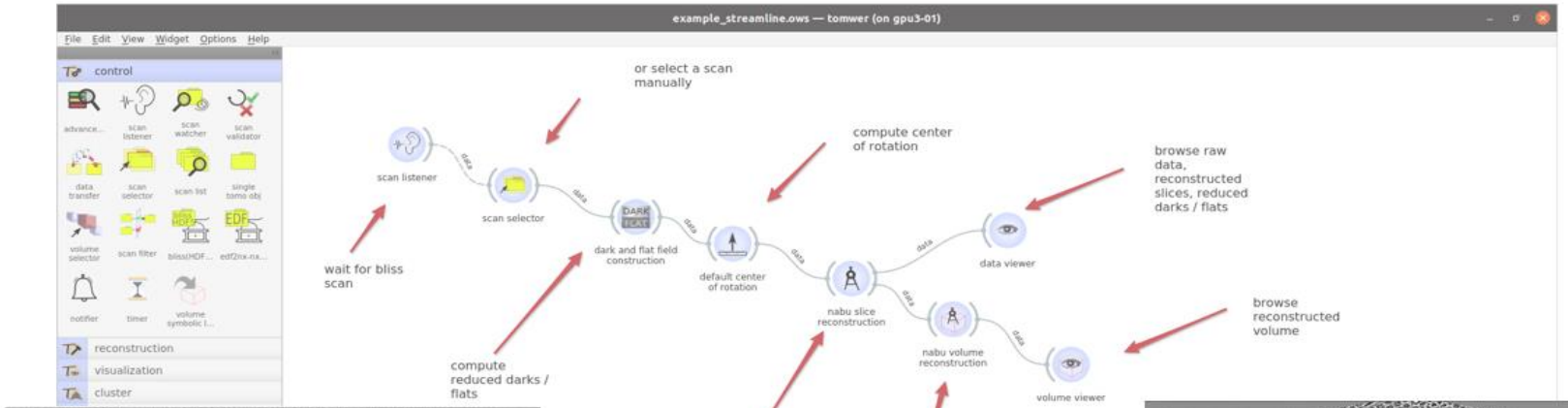
H5py like API for transparent on- and offline data access

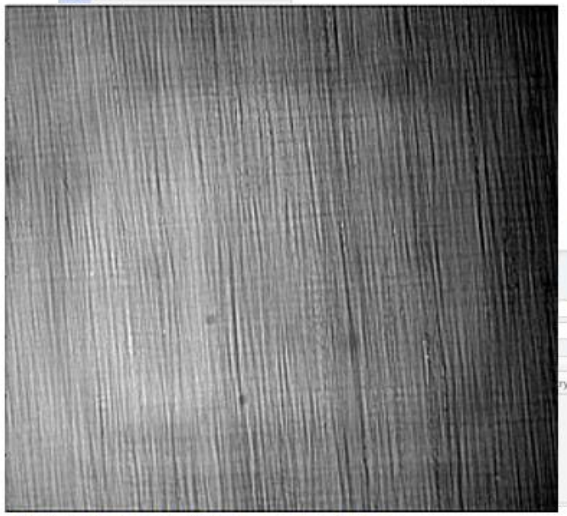
- The API switches transparently to file access when data is no longer available online

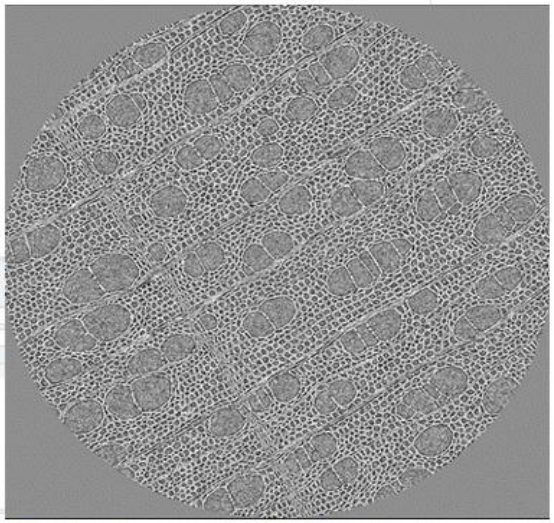


ONLINE DATA ANALYSIS - EWOKS

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





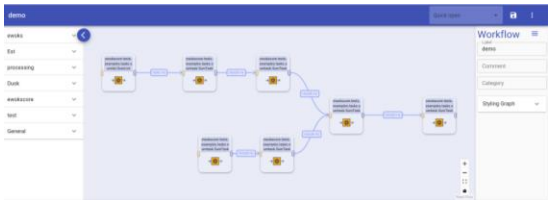


Inputs: BLISS scan data
(darks, flats, projections + metadata)

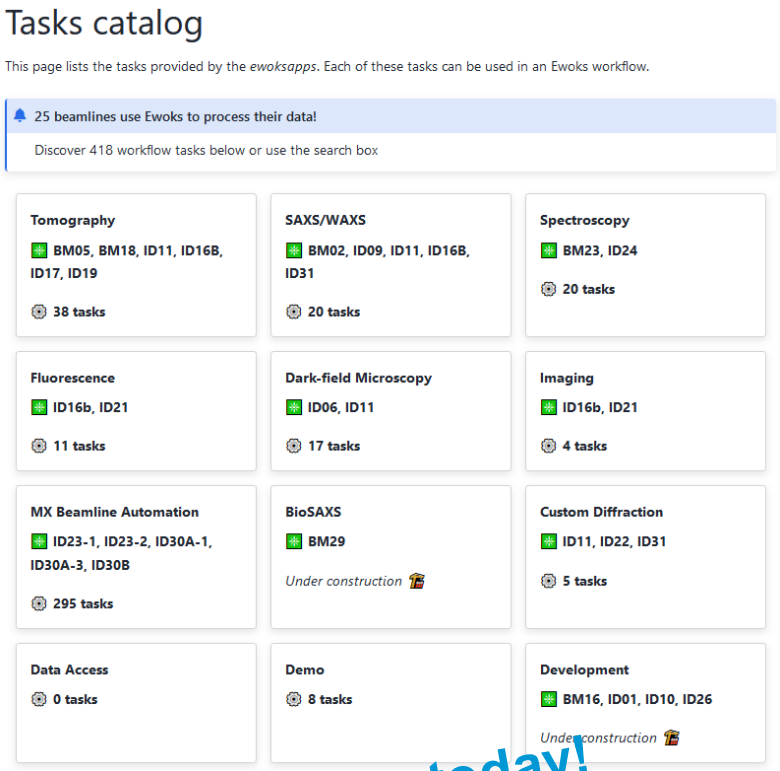
Outputs: reconstructed volumes

Workflow System for Online Data Analysis and Reduction

- Graphical chaining of predefined processing tasks by the user
- Web GUI to build workflows



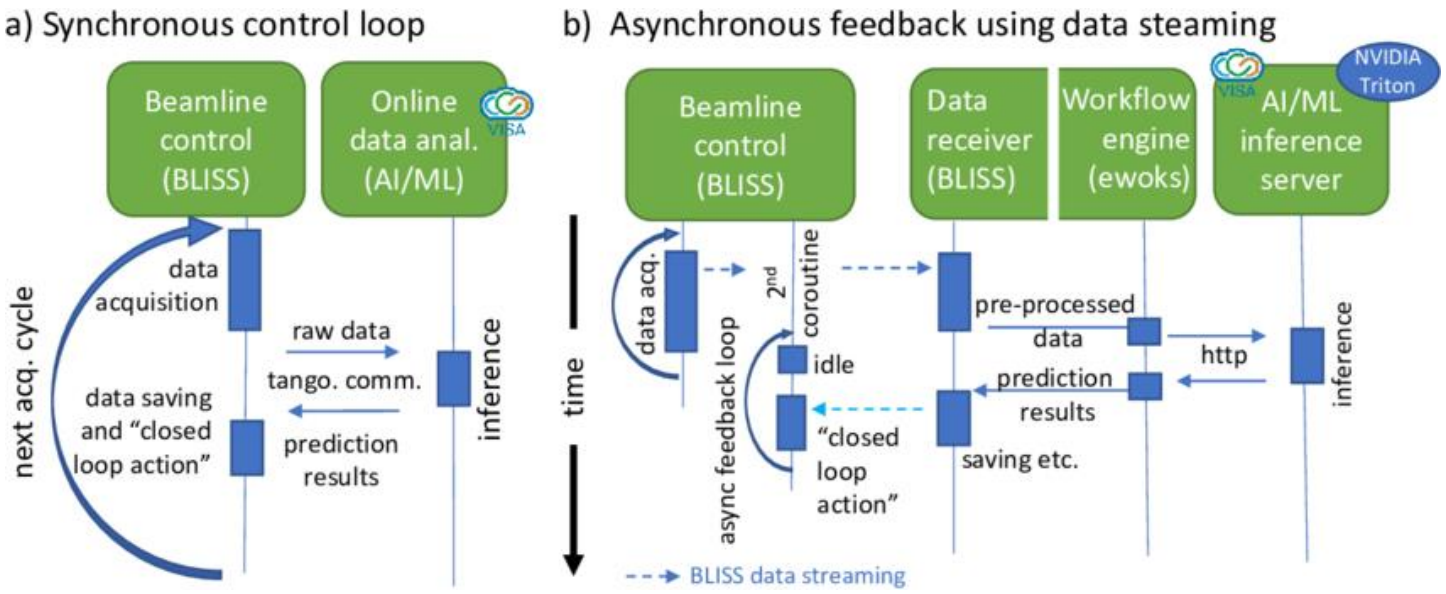
- Specific workflow tasks for every scientific domain
- Can run fully automated or manually
- Processing by CPU or GPU, locally or batch cluster
- Results can be stored or fed back to the acquisition system



EWOKS is running in daily operation on 25 beamlines today!

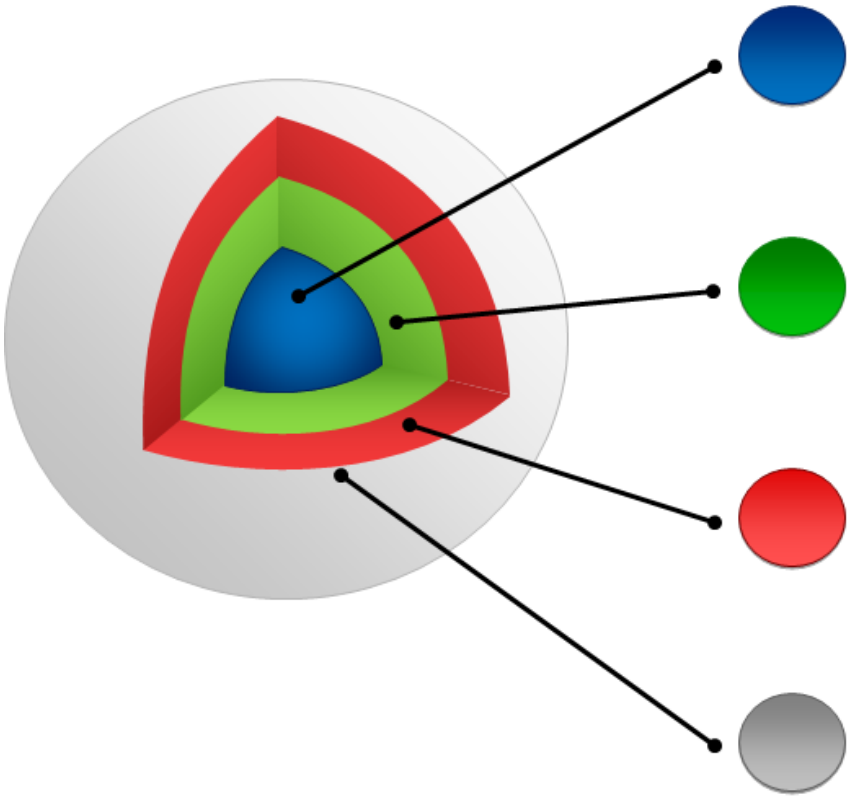
With BLISS and EWOKS the door is wide open for complex experiments

Example on ID10: Using AI/ML to close the loop with the running experiment



L.Pithan - Closing the loop: Autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments

FAIR DATA



DATA

The core bits

At its most basic level, data is a bitstream or binary sequence. For data to have meaning and to be FAIR, it needs to be represented in standard formats and be accompanied by Persistent Identifiers (PIDs), metadata and code. These layers of meaning enrich the data and enable reuse.

IDENTIFIERS

Persistent and unique (PIDs)

Data should be assigned a unique and persistent identifier such as a DOI or URN. This enables stable links to the object and supports citation and reuse to be tracked. Identifiers should also be applied to other related concepts such as the data authors (ORCIDs), projects (RAIDs), funders and associated research resources (RRIDs).

STANDARDS & CODE

Open, documented formats

Data should be represented in common and ideally open file formats. This enables others to reuse the data as the format is in widespread use and software is available to read the files. Open and well-documented formats are easier to preserve . Data also need to be accompanied by the code use to process and analyse the data.

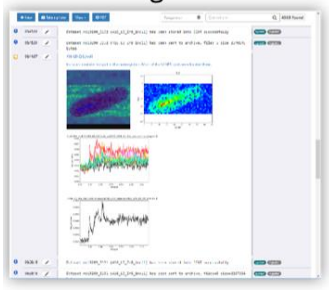
METADATA

Contextual documentation

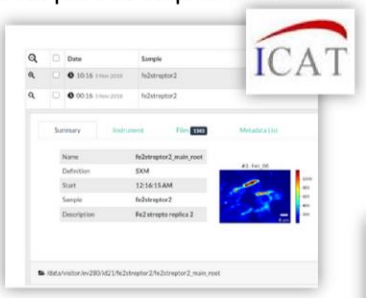
In order for data to be assessable and reusable, it should be accompanied by sufficient metadata and documentation. Basic metadata will enable data discovery, but much richer information and provenance is required to understand how, why, when and by whom the data were created. To enable the broadest reuse, data should be accompanied by a 'plurality of relevant attributes' and a clear and accessible data usage license.

Integration within the ESRF Ecosystem

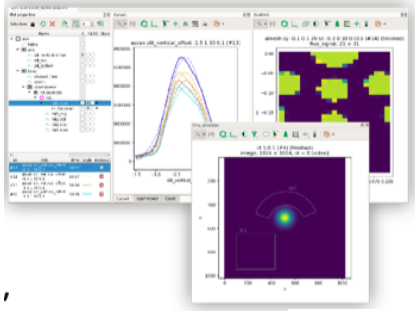
E-logbook



Data portal: https://data.esrf.fr

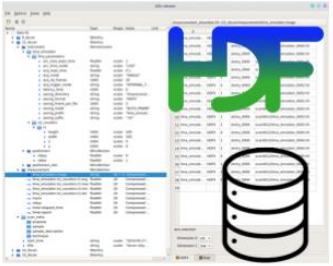


Live data visualization



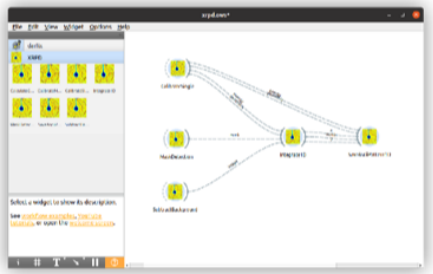
Experiment scripts, user sequences

Bliss



Efficient data format, storage

Online data analysis workflows

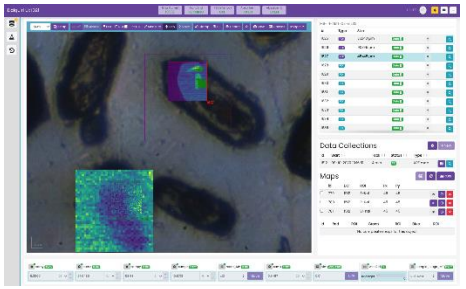


Sample changers, automation

Jungfrau @ ID29

Faster detectors, data production

Experiment GUIs



CONCLUSION

BLISS

- Ready to push-up the data acquisition frequency
- Easy integration of user software
- High flexibility to prepare complex experiments
- Online data visualization
- HDF5 saving structure, following the ESRF data policy, for all experiments
- Transparent online and offline data access for data analysis
- Decoupled data producers and data consumers. The BLISS data API can easily filled other data producers to use the same data analysis tools

EWOKS

- Workflow definitions for different science domains
- Easy automation of data reduction and online processing
- Result feedback to the running acquisition

THANK YOU

Acknowledgements to

- The members of the software group for the development of all the different software tools
- Our colleagues from the Technical Infrastructure Division for their work on the network and data storage infrastructure
- All the beamline scientists for their feedback, patience and bug reports since the EBS start-up