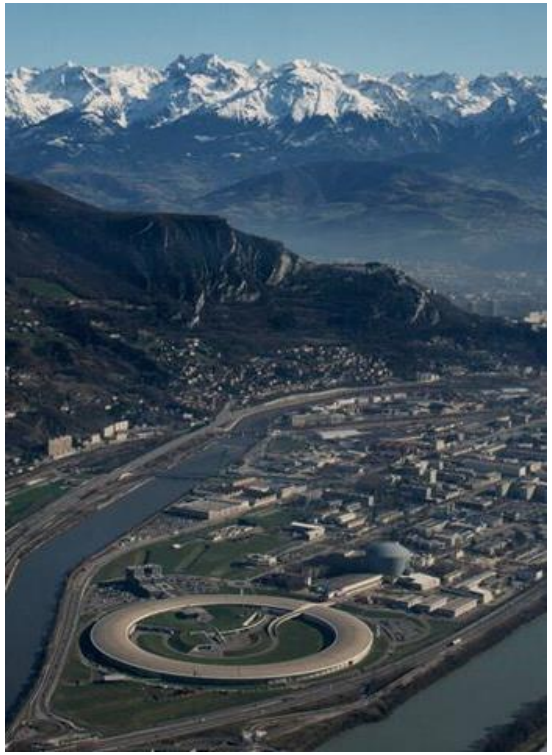

ESRF
The European Synchrotron

REMOTE USER OPERATION OF ESRF EXPERIMENTS

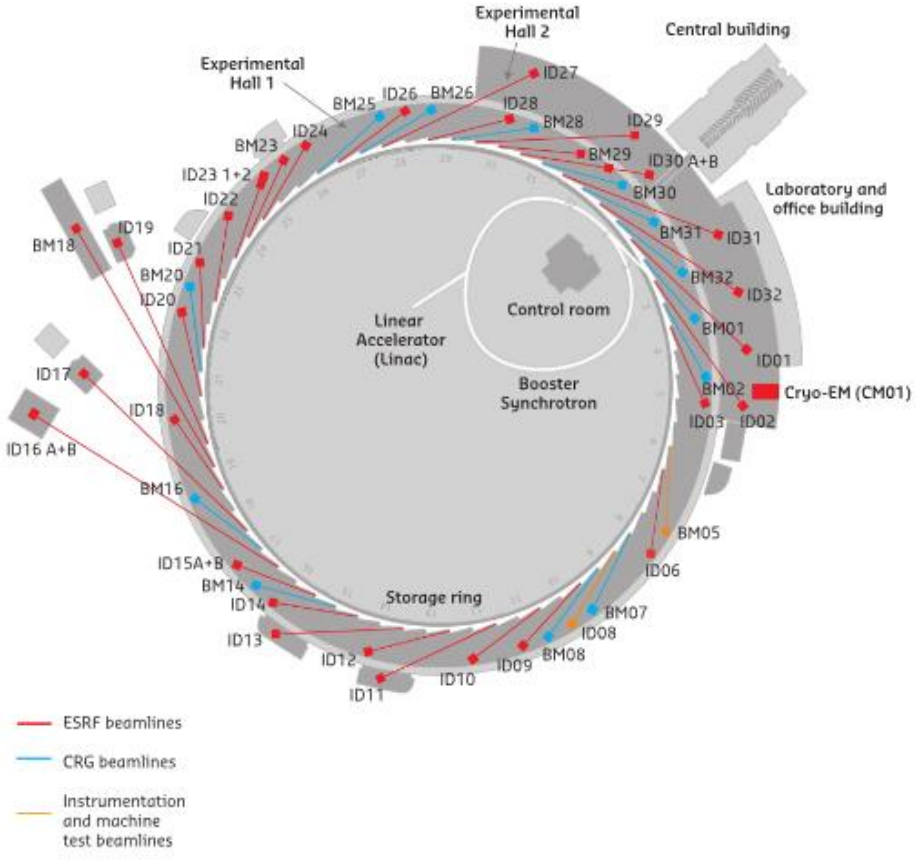


Outline

- A Global view
- Remote Experiments Step by Step
- On-going work

Jens Meyer on behalf of the ESRF Software Group

ESRF Beamlines and Experiment Types



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

A GLOBAL VIEW

Operation until 2018:

Users come to the ESRF and bring their samples

Users execute their experiments on-site and intervene in the hutches

Users transfer small amounts of data via the network or bring their own disks for large data volumes

Only structural biology beamlines are automated for remote operation

Operation since 2020

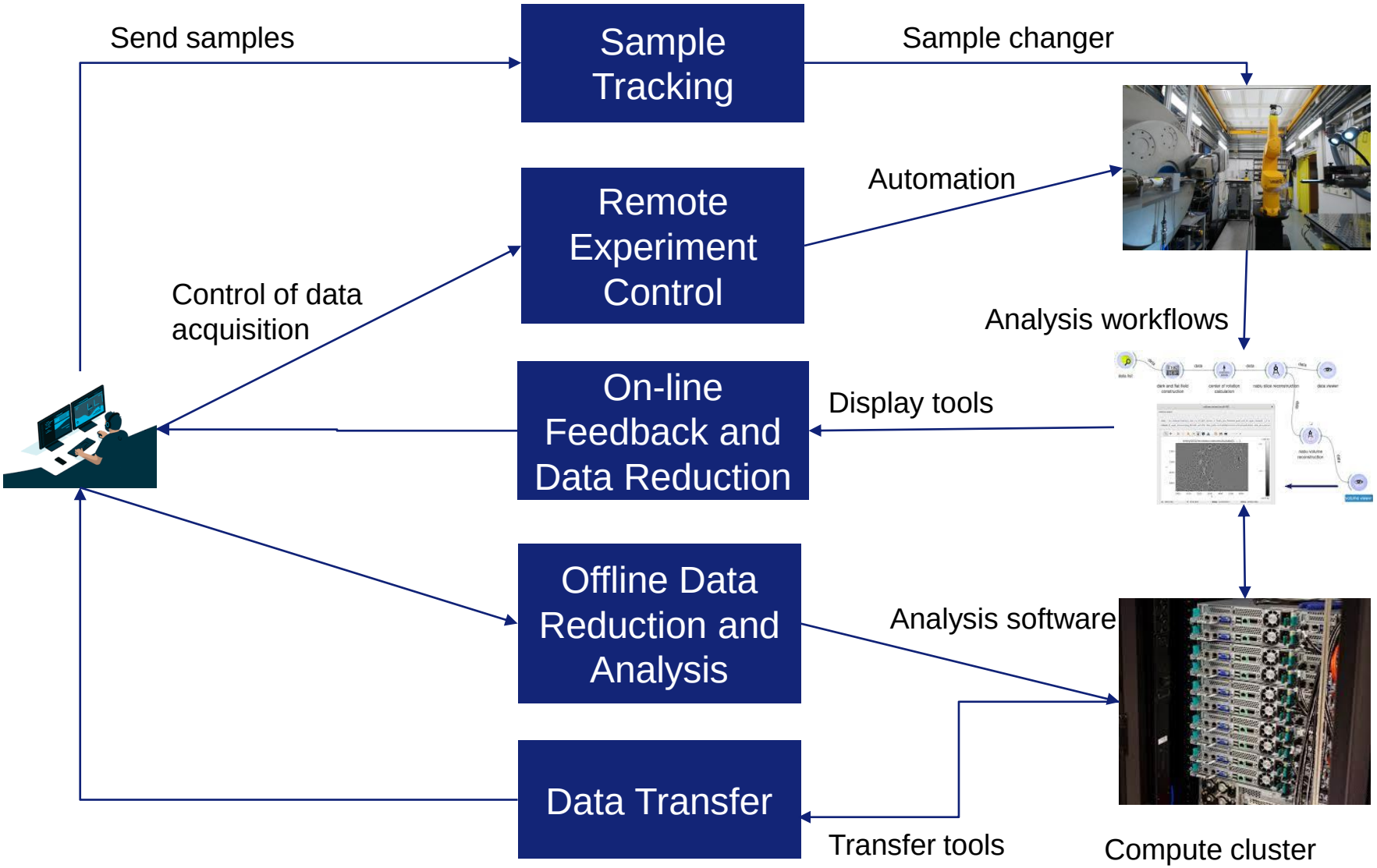
Commissioning of the new storage ring (EBS)

- More photons -> faster experiments and more raw data
- Data analysis needs more compute power
- Large raw data sets are more difficult to transfer (up to 100TB)

COVID restrictions -> No users on site

- Remote operation of all beamlines to run the ESRF
- Remote operation with different levels of automation
- Operation with limited local staff
- A fast solution for remote user operation was requested

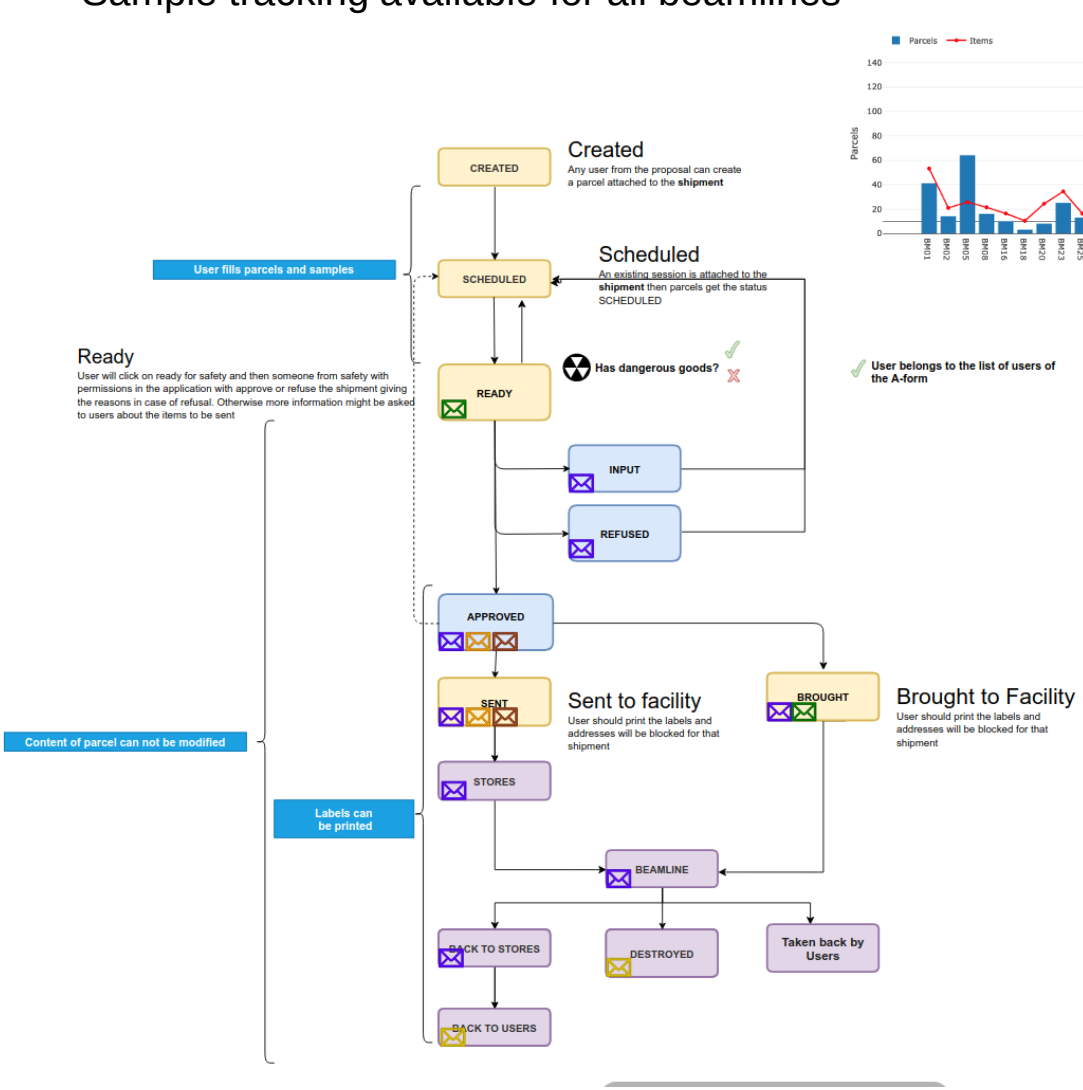
A GLOBAL VIEW

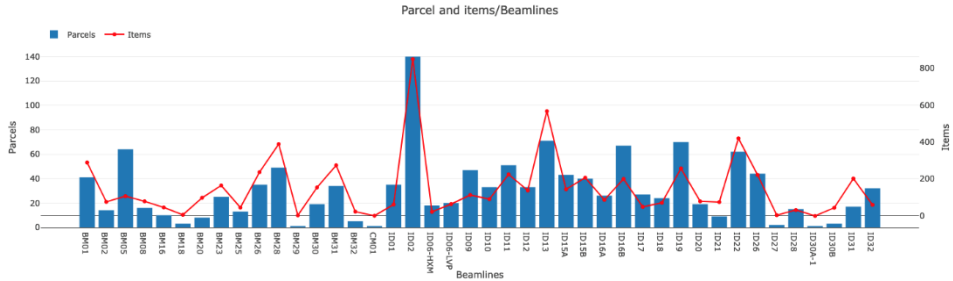


SAMPLE TRACKING

Known from Structural Biology beamlines

Sample tracking available for all beamlines





User belongs to the list of users of the A-form

LEGEND

- Notification to expsaf@esrf.fr if contains dangerous goods
- Notification to safety group (expsaf@esrf.fr)
- Notification to users
- Notification to users, local contact and BDO (industry@esrf.eu) in case of IM/IN
- Notification to esrftransport@esrf.fr
- Notification to users and BDO (industry@esrf.eu)in case of IM/IN

Action done by users

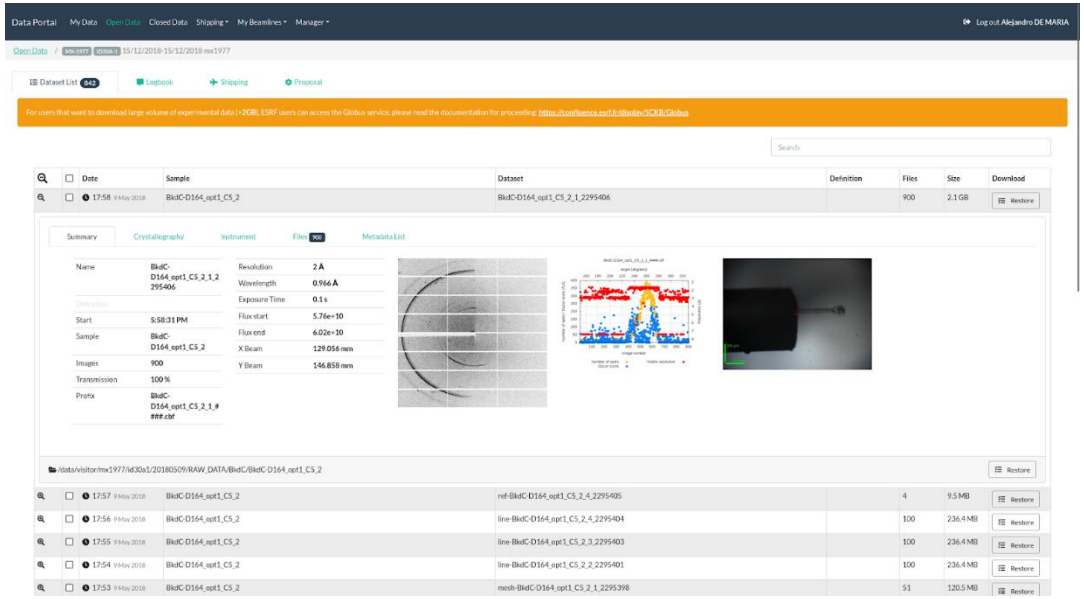
Action done by safety

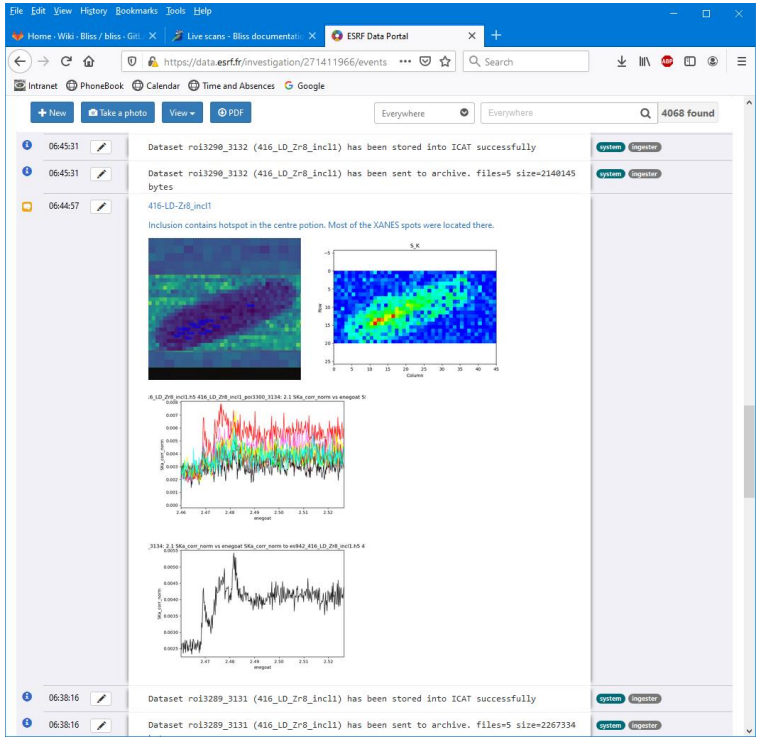
Action done by staff (stores or local concatcts)

DATA ACQUISITION

Automation

- Sample changers (local staff cannot always be available to intervene in the hutch)
- High level data acquisition sequences
- Flexibility to allow users or local staff to adapt the data acquisition
- Standardized data format and data organization
- Experiment registration with meta data and electronic logbook (web applications)





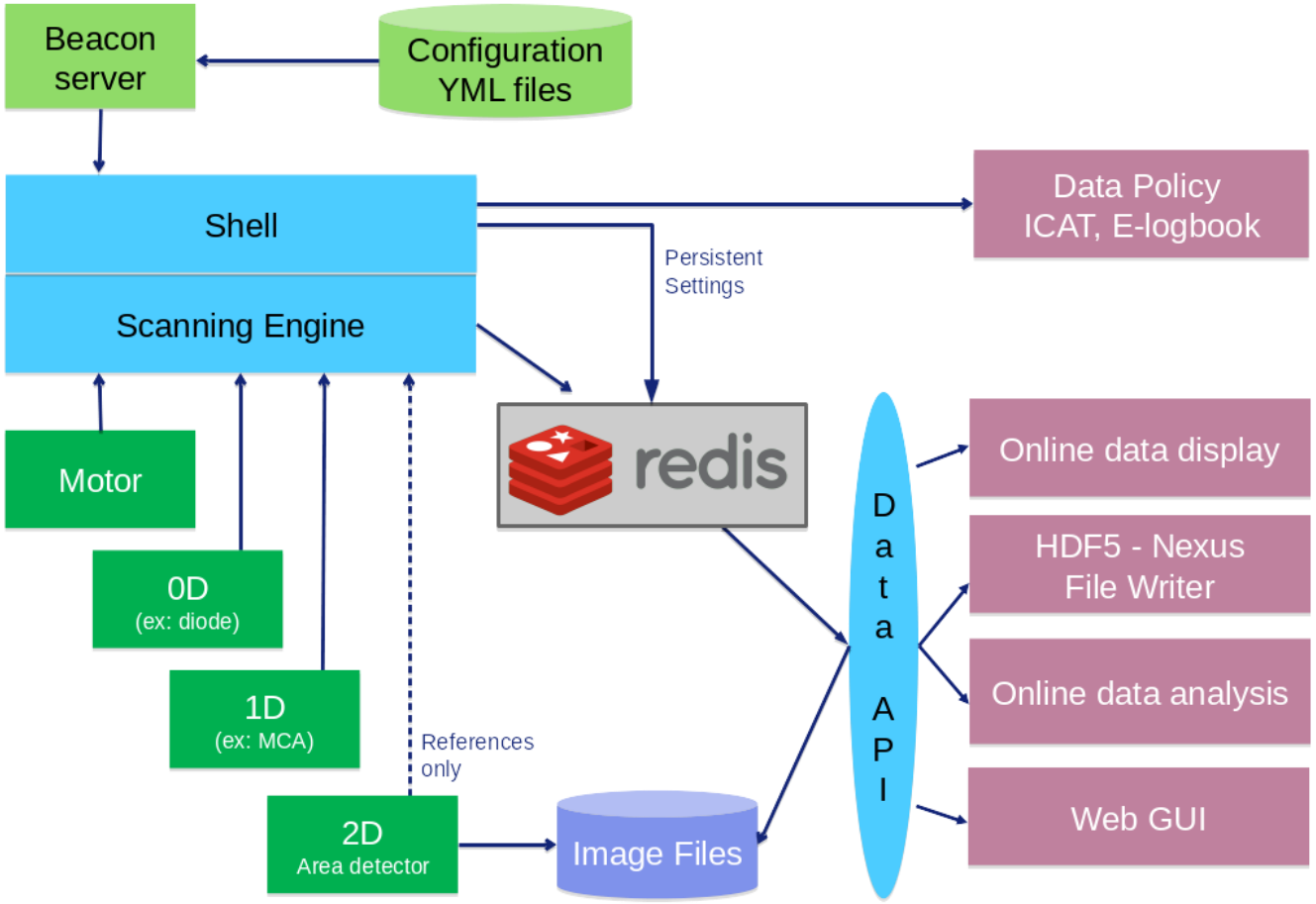
ICAT

Bliss architecture and data flow

Experiment sequences written in pure python

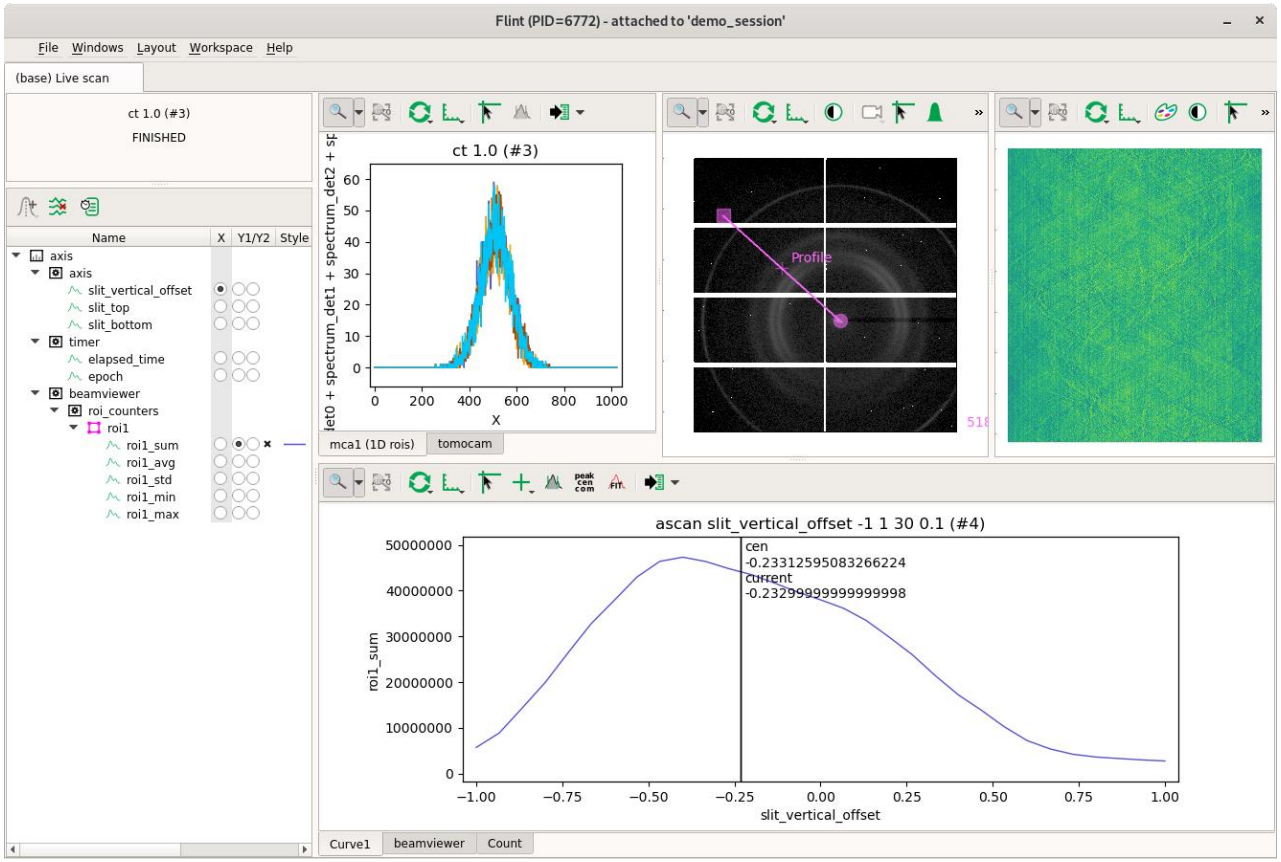
Unified scanning engine for step and continuous scans

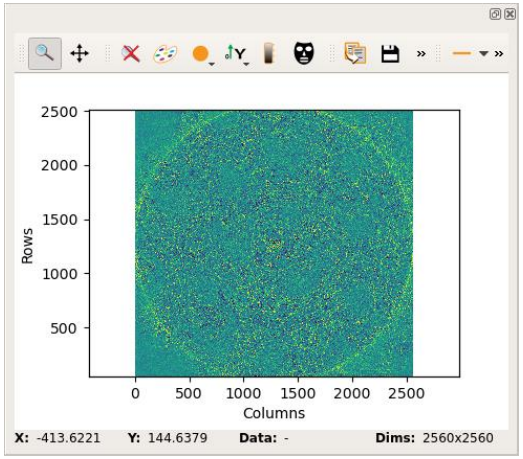
Scan data and meta data saving in HDF5 file format following the NeXus definitions

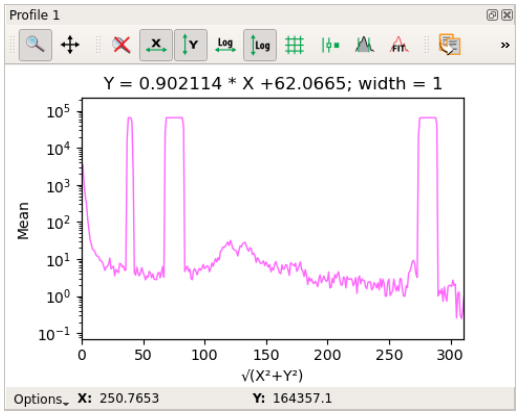


Bliss architecture and data flow

Live data display







Remote operation for all beamlines

Not all GUIs are web application

Heavy use of the command line interface

Remote desktop to the beamline control workstations

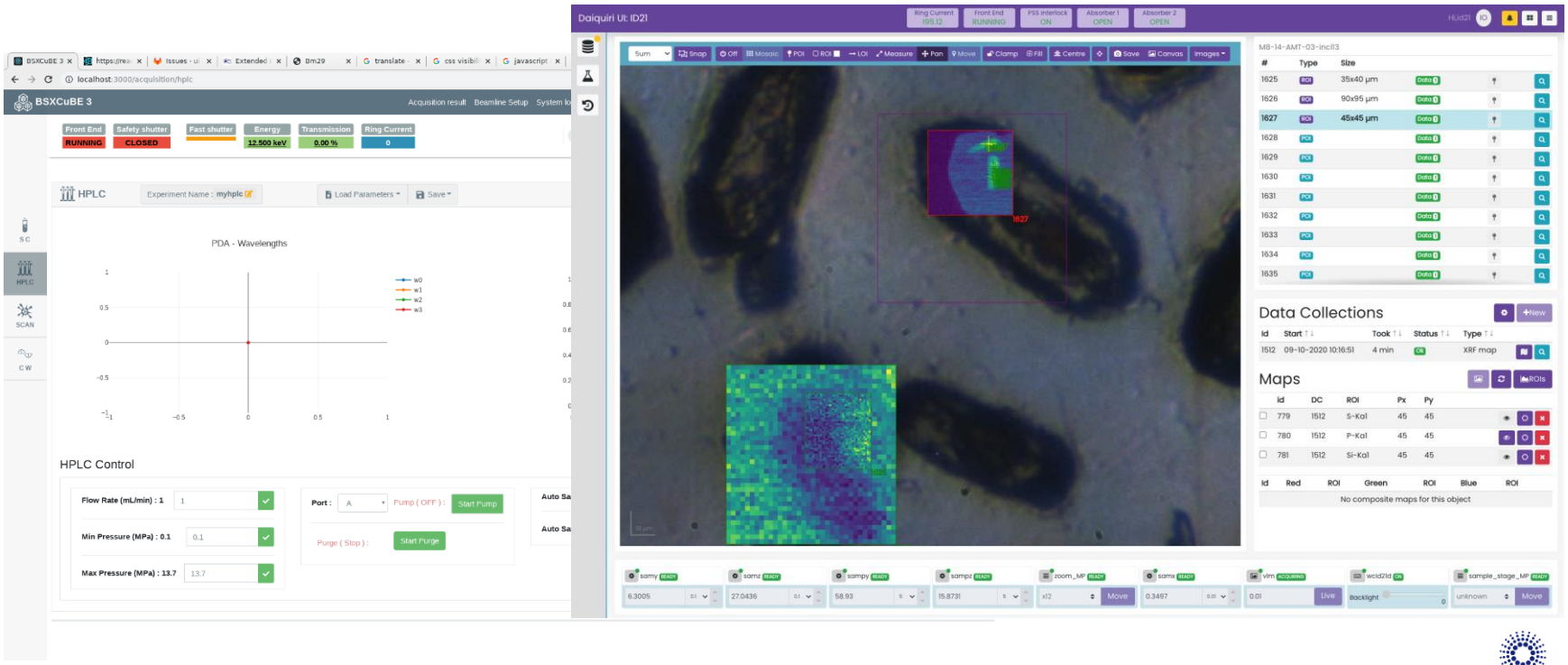
- Guacamole for desktop sharing
  - > *Multiple screens*
  - > *Multi connections*
- Zoom for direct communication

Remote operation for fully automated experiments

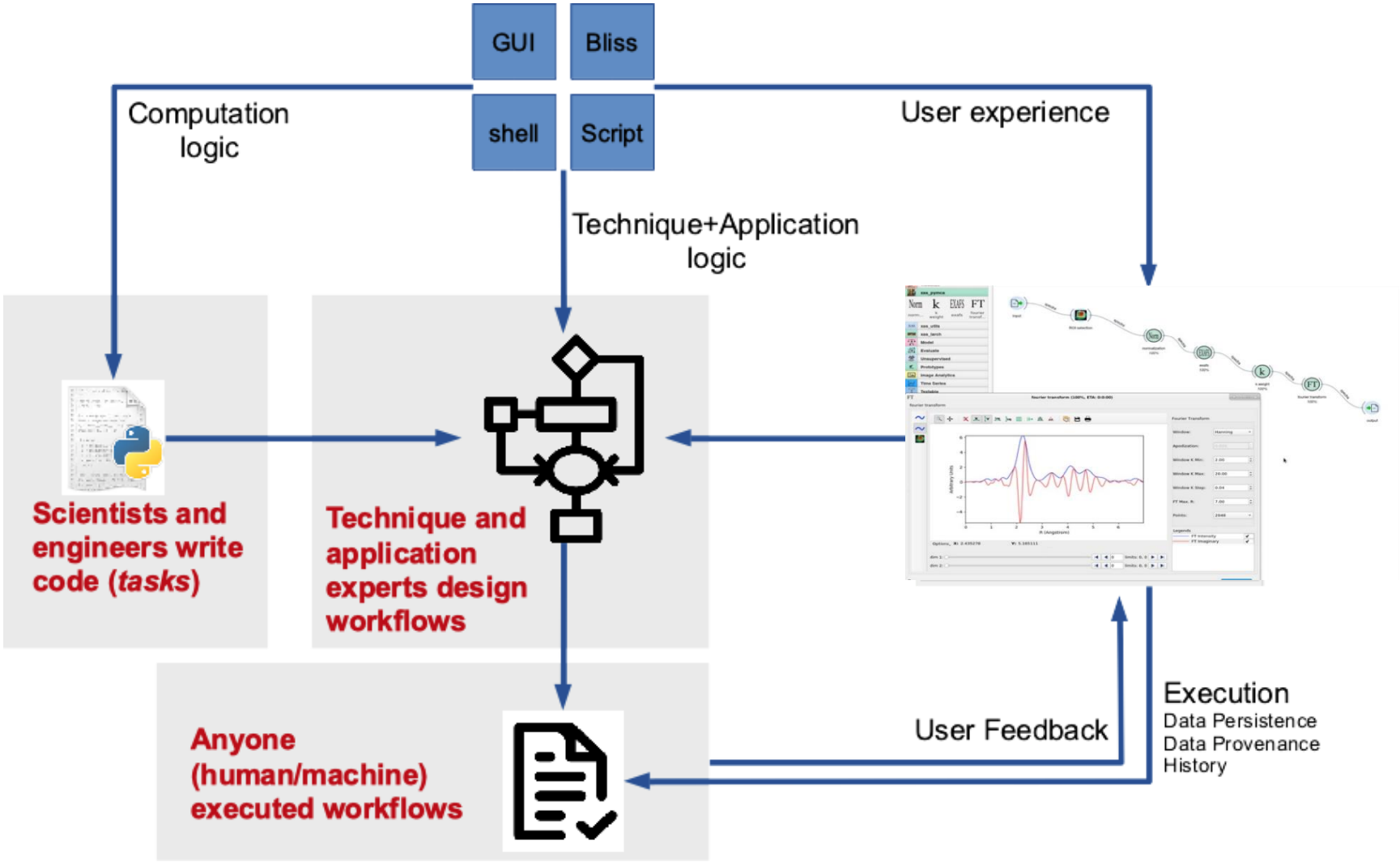
Web GUIs

- Experiment control
- On-line feedback
- Pre-analysis for data validation
- Data reduction

} Data processcing workflows



Data Processing Workflows



Data Processing Workflows

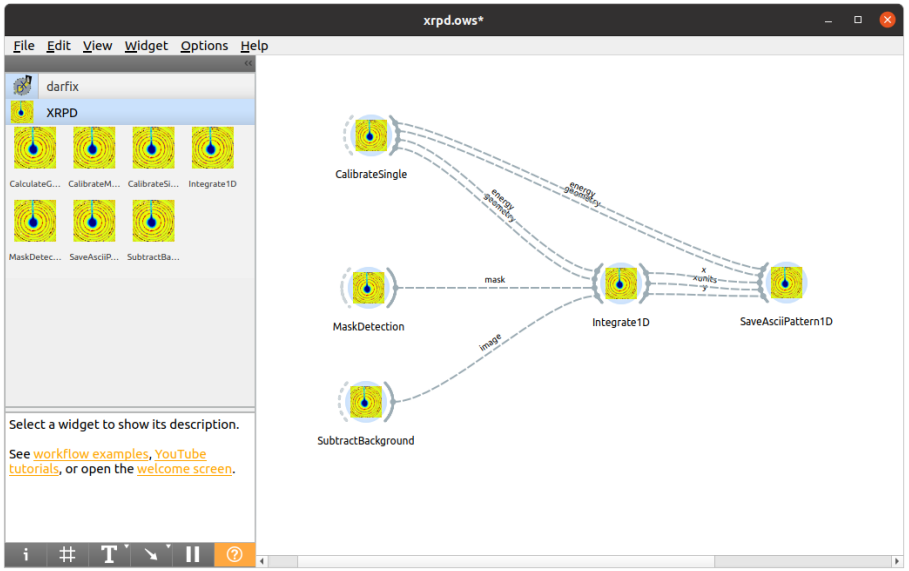
Ewoks

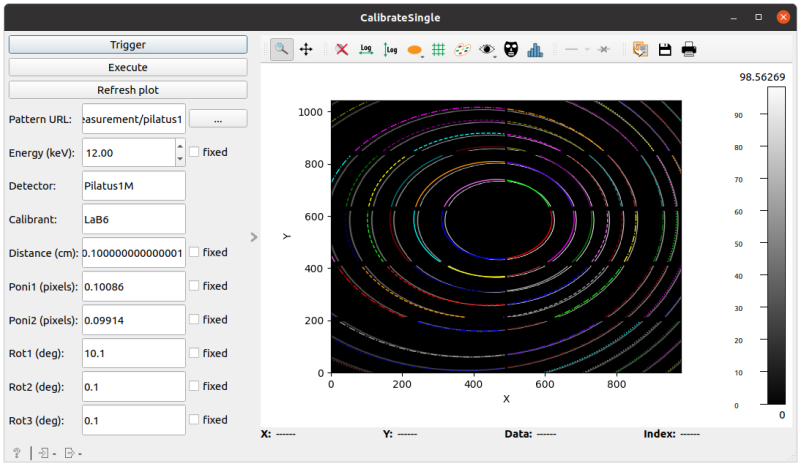
- Common workflow definition
- Common task definition
- Distributed execution (Dask, Slurm)
- Loops and conditions (pypushflow)
- Web GUI (Ewoksweb)
- Data persistence (HDF5, Redis)
- Execution events for client feedback

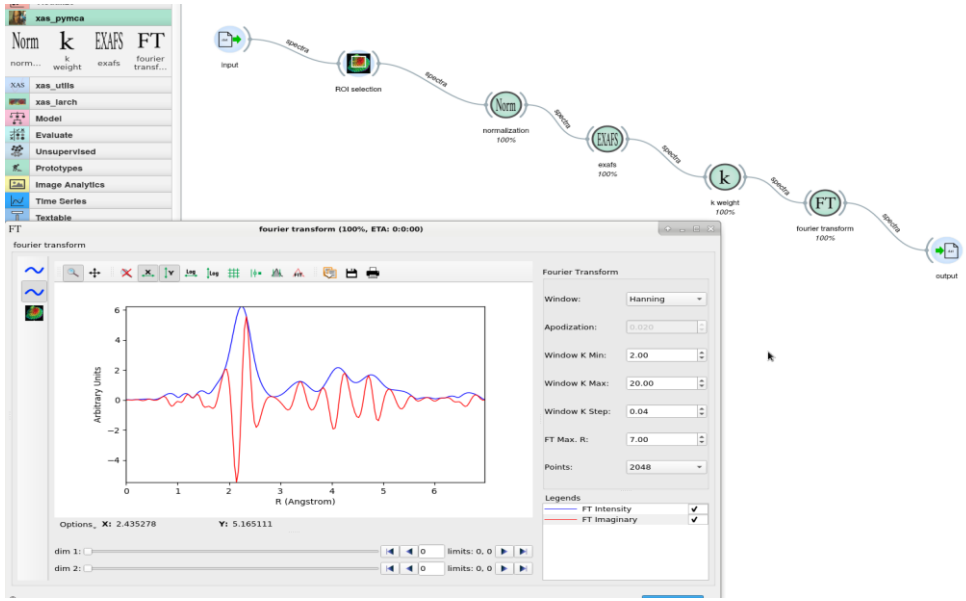
Projects

- Tomography (Tomwer)
- Darkfield microscopy (Darfix)
- MX (MASSIF-1)
- Spectroscopy (Est)
- EASI-STRESS (stress-strain analysis)
- STREAMLINE High-Throughput XRPD

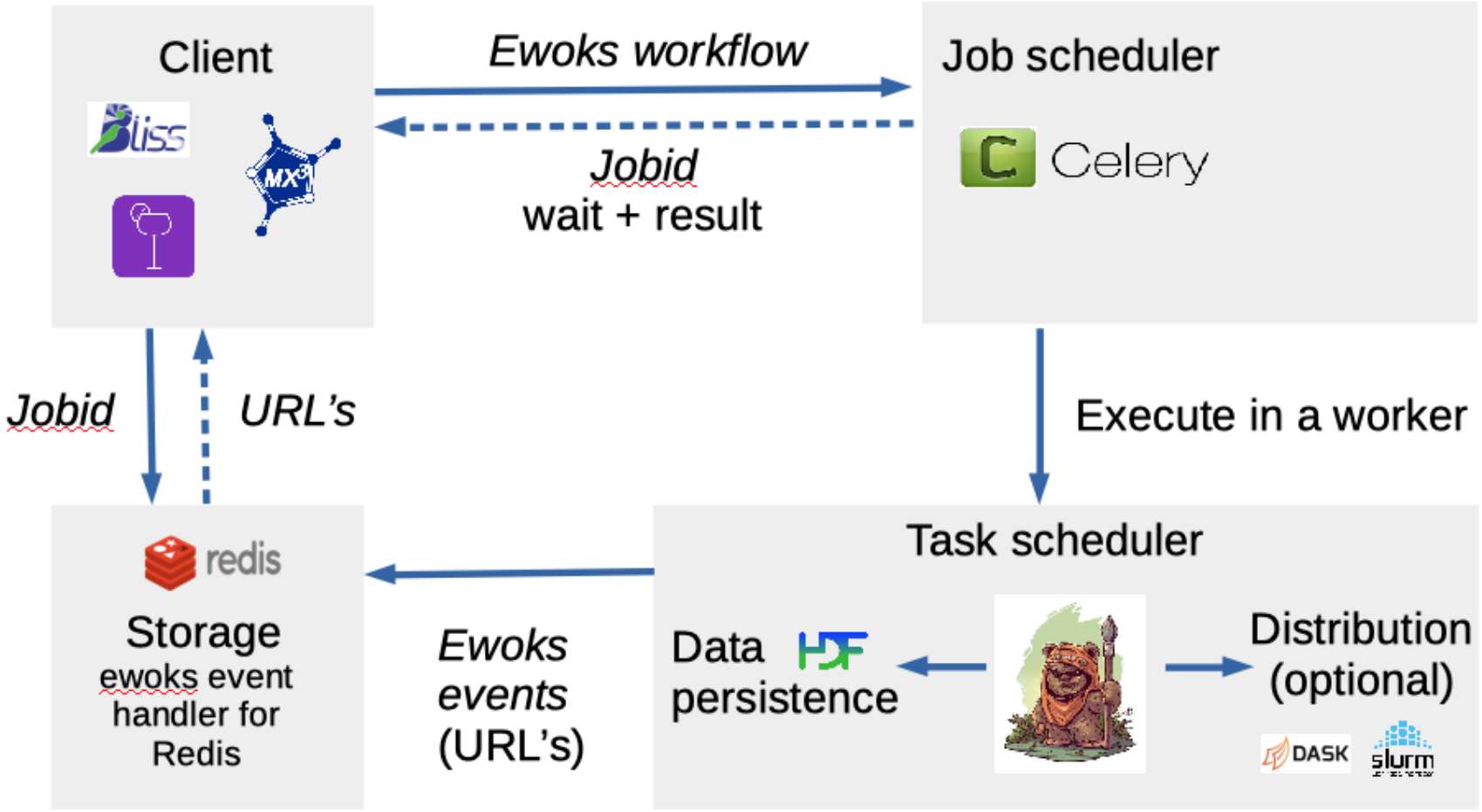
DATA REDUCTION AND ONLINE ANALYSIS





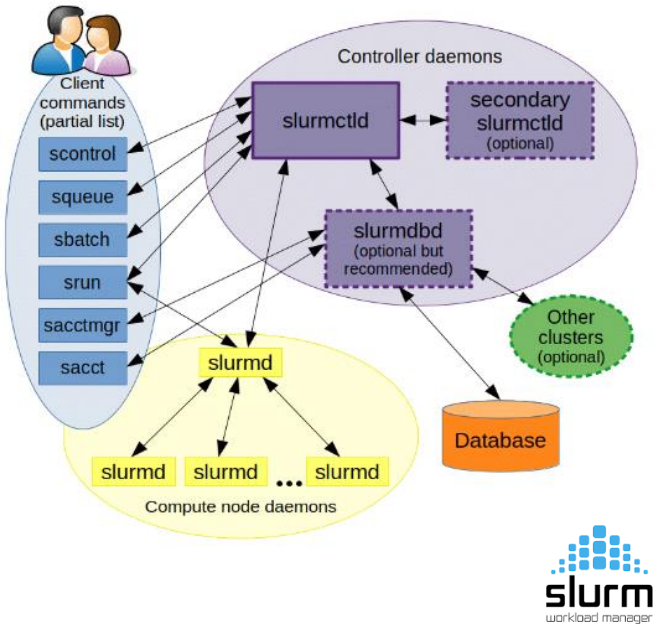


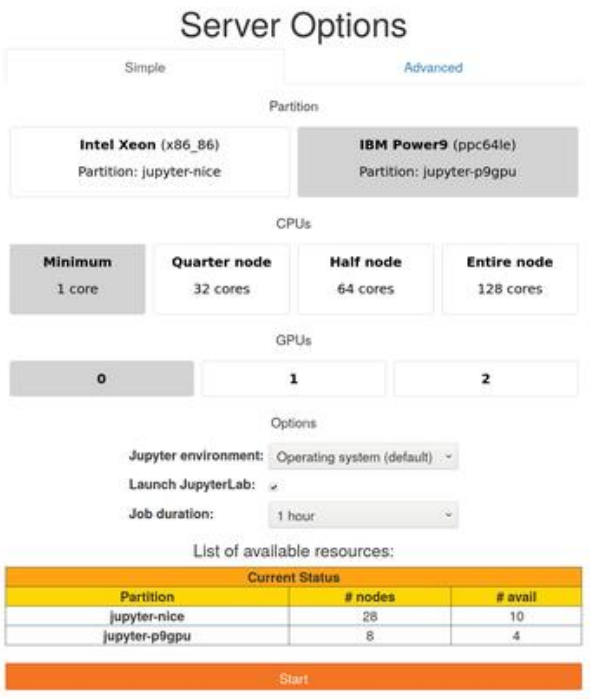
Woks for Online Data Processing



Remote data analysis at the ESRF

- Large data sets are difficult to transfer
- Need of optimized analysis software
- Need of a powerfull computing infrastructure
- Remote data analysis needs specific infrastructure to handle users and resources
  - *Jupiter notebooks on Slurm*





Higher degree of automation in data acquisition and analysis

- Need more standardization of the different experiment types
  - *Definition of the experimental sequence, the options and the parameters*
  - *Better standardization of the data structure produced*
  - *Adapted data analysis software*
  - *Agreement on data processing workflows*
- Efficient data reduction and pre-analysis
  - *Users should keep only the reduced data*
  - *Be sure data contains useful information*
- HPC computing for analysis at ESRF
  - *Enlarge the infrastructure for remote access*
  - *Make more data analysis software available*
  - *Increase the computing resources*

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 computing infrastructure
- All the beamline scientists for their patience and problem reporting since the EBS startup.