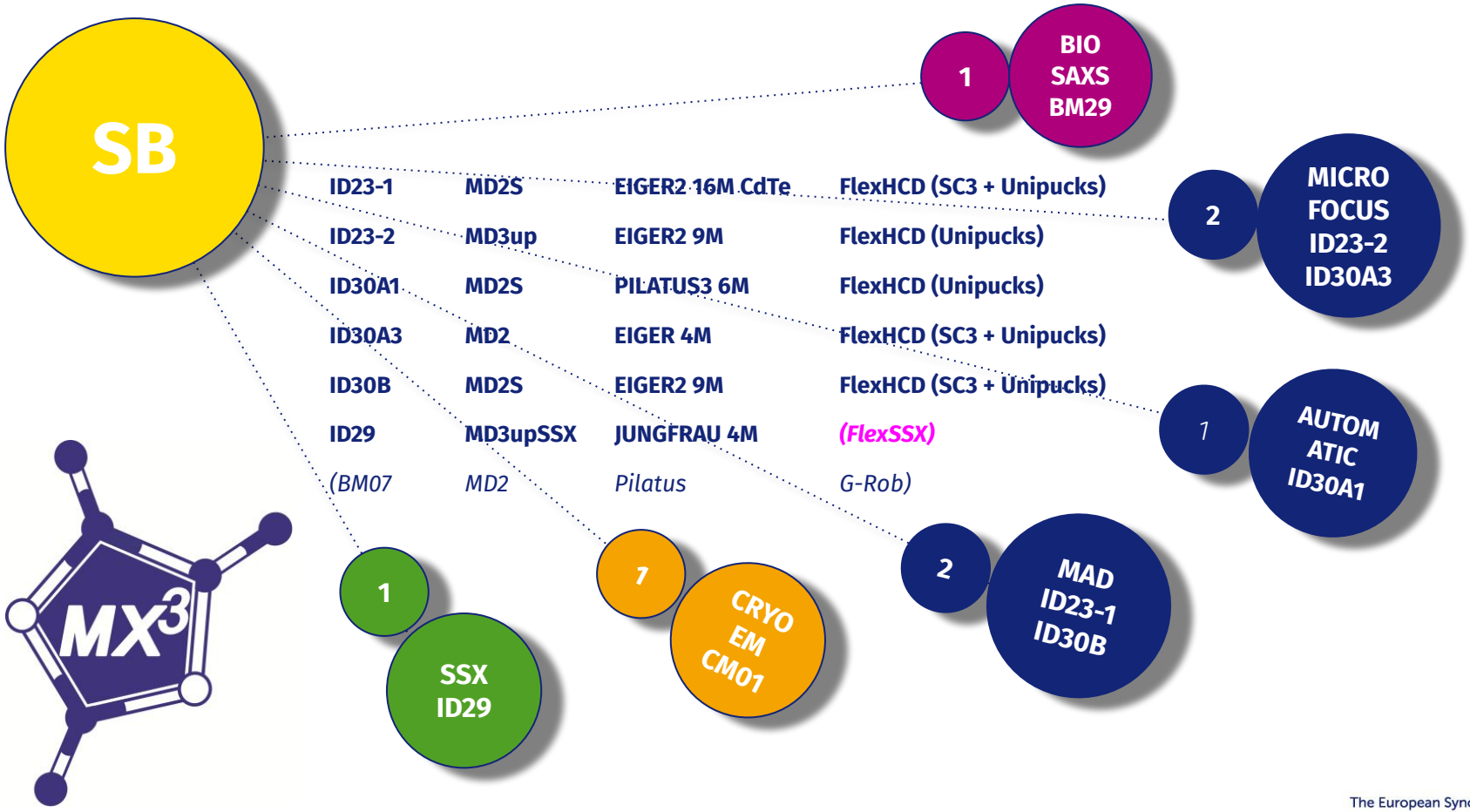
ESRF Status Report

Daniele de Sanctis

On behalf of the rest of the team:
Marcus Oscarsson, Antonia Beteva, Olof Svensson, Axel Bocciarelli, Jean Baptiste Florial (*EMBL*) and the SB-Group

OVERVIEW


SB
1
BIO
SAXS
BM29
ID23-1 MD2S EIGER2 16M CdTe FlexHCD (SC3 + Unipucks)
ID23-2 MD3up EIGER2 9M FlexHCD (Unipucks)
ID30A1 MD2S PILATUS3 6M FlexHCD (Unipucks)
ID30A3 MD2 EIGER 4M FlexHCD (SC3 + Unipucks)
ID30B MD2S EIGER2 9M FlexHCD (SC3 + Unipucks)
ID29 MD3upSSX JUNGFRAU 4M (FlexSSX)
(BM07 MD2 Pilatus G-Rob)
2
MICRO
FOCUS
ID23-2
ID30A3
1
AUTOM
ATIC
ID30A1
2
MAD
ID23-1
ID30B
1
CRYO
EM
CM01
1
SSX
ID29
MX3

CURRENT STATUS

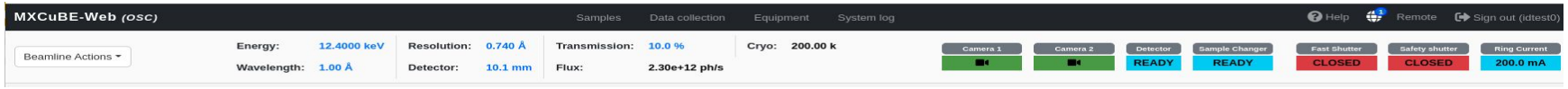
- MXCuBE Web 3 on ID23-2 and MASSIF3
  - MX beamlines are running almost completely remotely
- MXCuBE Web 4 with mxcubecore deployed in production on
  - ID29 For SSX experiments
  - ID30A1 For Automatic data collection, Harvester and Plate integration
  - ID23-1 Mainly proprietary research now
  - ID30B currently commissioning
  - ID23-2 during winter shutdown
- BSXCuBE3 on BM29
- Since last MXCuBE meeting
  - Initial Pump&probe experiments on ID29
  - Implementation of in-situ (plates) experiments on MASSIF1 (N.Foos)
  - Deployment of GPhL workflows
  - Developments on ID23-1 to increase sample throughput

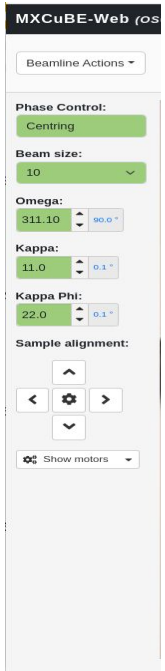
MXCUBE WEB 4

- MXCuBE Web 4
  - Based on **mxcubecore**
  - Major Backend and frontend library **updates**
  - New **sample view**
  - **In situ** data collection
  - **Configurable display**
  - **Braggy** and heatmap integration
  - **SSX** modes for ID29

  - Adding **Methods** and procedures in three ways:
    - **Equipment view** - For not so often used or temporary instrumentation commands
    - **Beamline action** - For procedures that are frequently used and involves more than a simple command
    - **Queue entry / task** - For collecting data

MXCUBE WEB 4 - CONFIGURABLE DISPLAY





The display of available instrumentation is configurable in ui.yaml

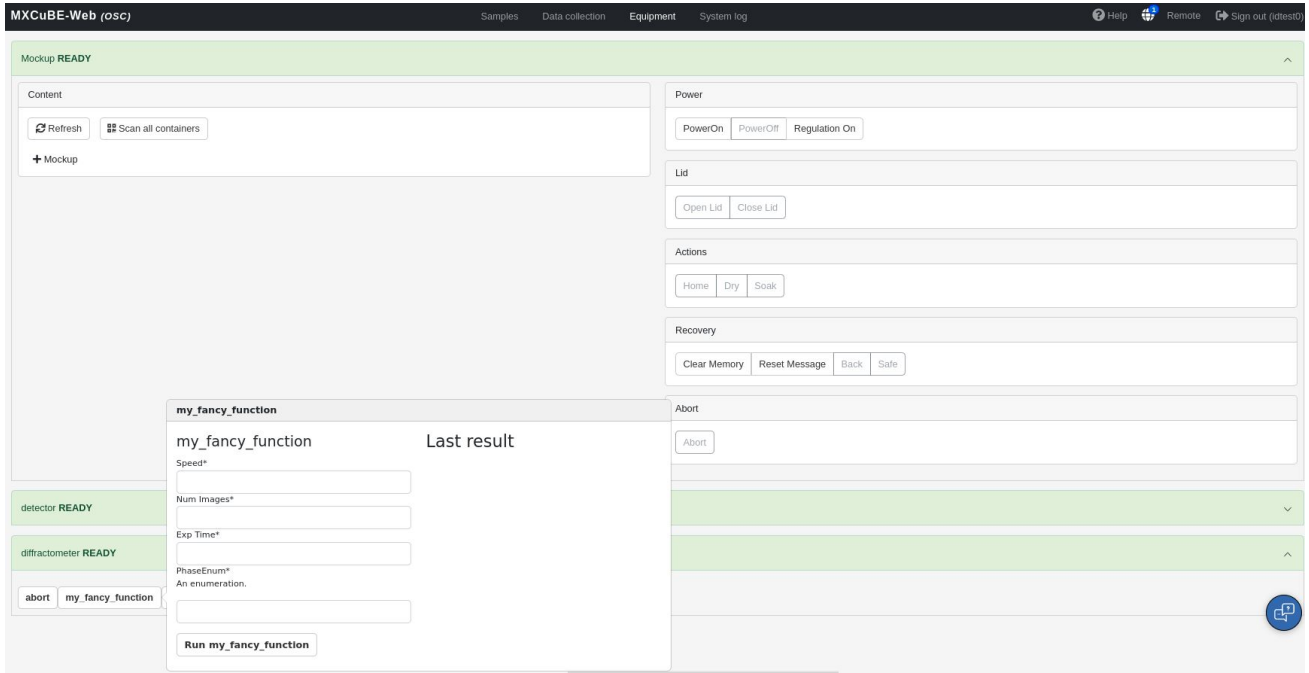
To the left motor control and on the top “beamline setup”

```yaml
sample_view:
  id: sample_view
  components:
    -
      label: Omega
      attribute: diffractometer.phi
      role: omega
      step: 90
      precision: 2
      suffix: °
    -
      label: Kappa
      attribute: diffractometer.kappa
      role: kappa
      step: 0.1
      precision: 1
      suffix: "°"
```

```yaml
beamline_setup:
  id: beamline_setup
  components:
    -
      label: Beamstop
      attribute: beamstop
    -
      label: Capillary
      attribute: capillary
    -
      label: Fast Shutter
      attribute: fast_shutter
    -
      label: Safety shutter
      attribute: safety_shutter
    -
      label: Detector
      attribute: detector
    -
      label: Energy
      attribute: energy
      step: 0.001
      precision: 4
      suffix: keV
```

MXCUBE WEB 4 - EQUIPMENT VIEW

Equipment view - For less often or temporary instrumentation commands

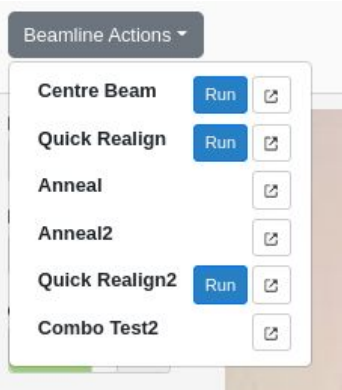


Methods are automatically added if they are “exported” with the export tag and the method is type hinted (at least with a return type)

```
<exports>["abort", "status", "my_fancy_function", "my_other_funny_function"]</exports>
```

Beamline action - For procedures that are frequently used and involves more than a simple command

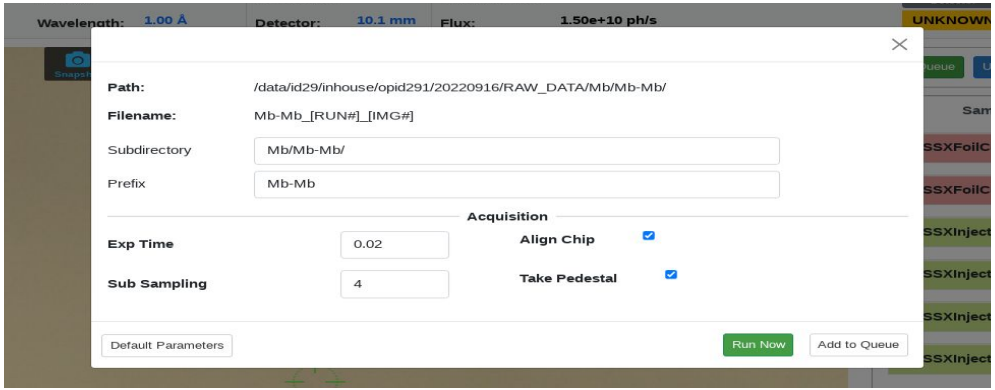
Configured as the beamline_actions of the Beamline hardware object




```
<object class="BeamlineActionsMockup">
    <commands>[
      {"type": "controller", "name": "Centre Beam", "command": "HardwareObjects.mo
      {"type": "controller", "name": "Quick Realign", "command": "HardwareObjects
      {"type": "controller", "name": "Anneal", "command": "HardwareObjects.mockup
      {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMoc
      {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMoc
      {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMoc
    ]
    </commands>
</object>
```


Marcus Oskarsson (marcus.oscarsson@esrf.fr)

Queue entry / task - For collecting data

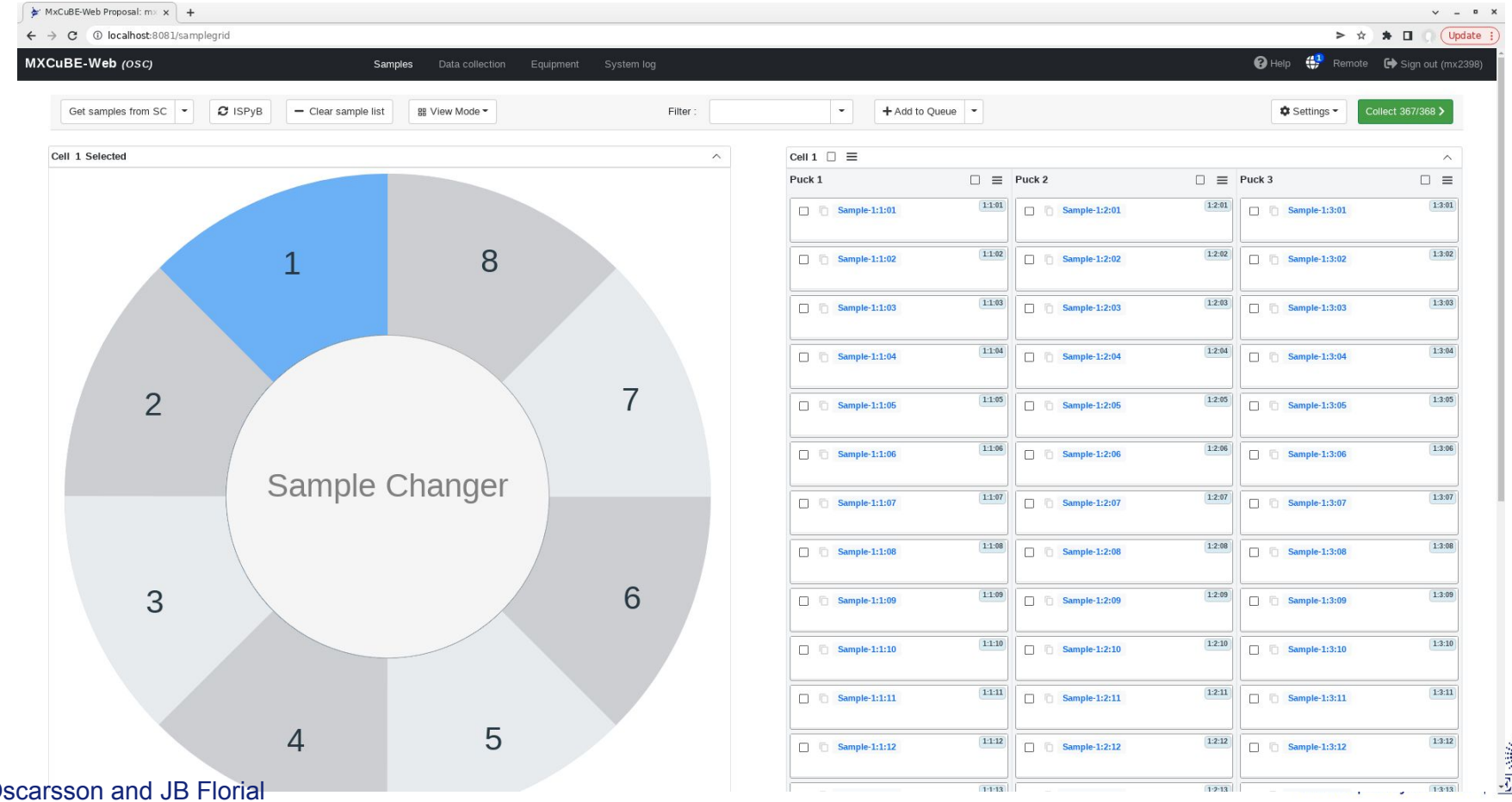


Write a task that takes a Pydantic model and add it to available_methods of Beamline object

```python
    legacy_parameters: LegacyParameters


class SsxChipCollectionQueueEntry(BaseQueueEntry):
    """
    Defines the behaviour of a data collection.
    """
    DATA_MODEL = SsxChipColletionTaskParameters
    NAME = "SSXChipCollection"
    REQUIRES = ["point", "line", "no_shape", "chip", "mesh"]

    # New style queue entry does not take view argument,
    # adding kwargs for compatability, but they are unsued
    def __init__(self, data: SsxChipColletionTaskParameters, view=None,
        super().__init__(view=view, data_model=TaskNode(data))


    def execute(self):
        super().execute()
```

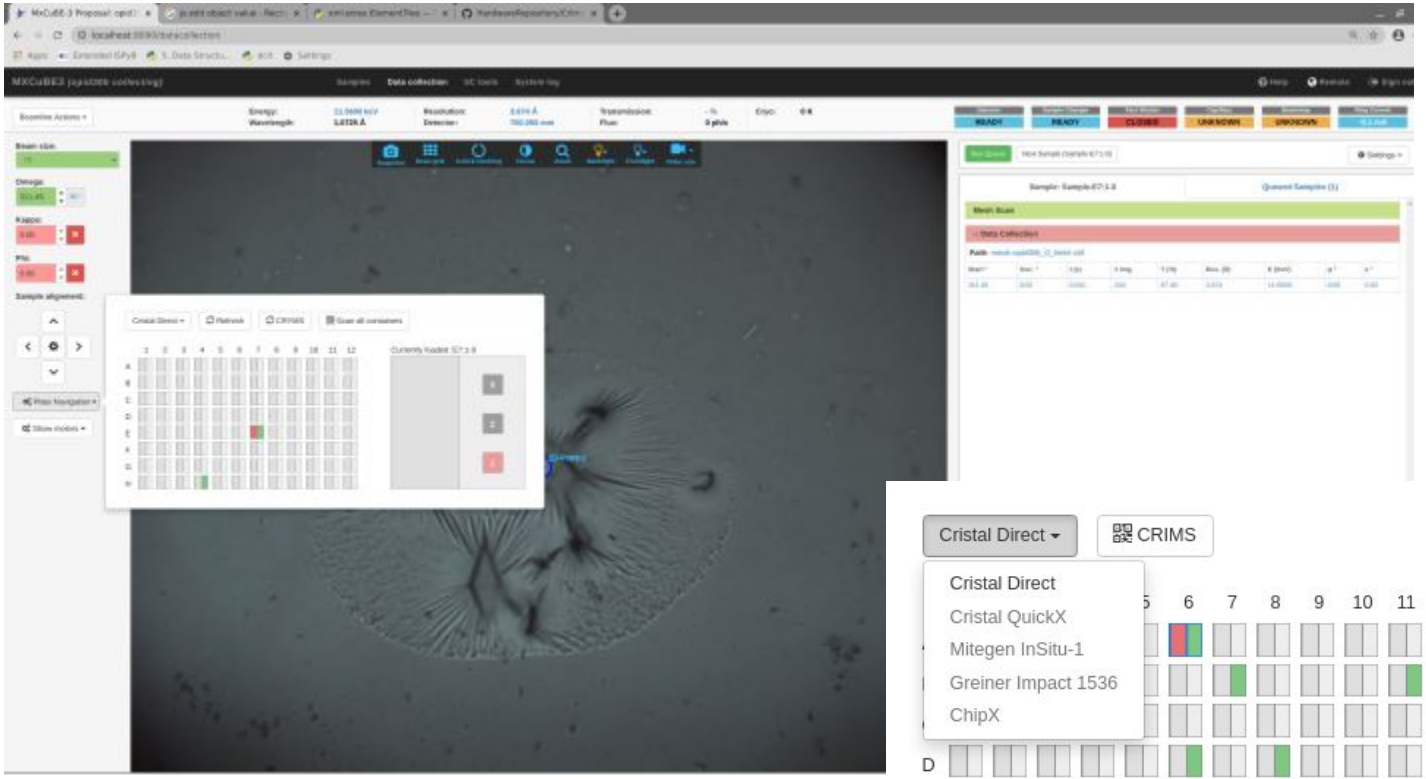
```yaml
available_methods:
    datacollection: True
    characterisation: True
    helical: True
    xrf_spectrum: True
    energy_scan: True
    mesh: True
    ssx_chip_collection: True
    gphlworkflow: True
    test_collection: True
```

NEW SAMPLES VIEW

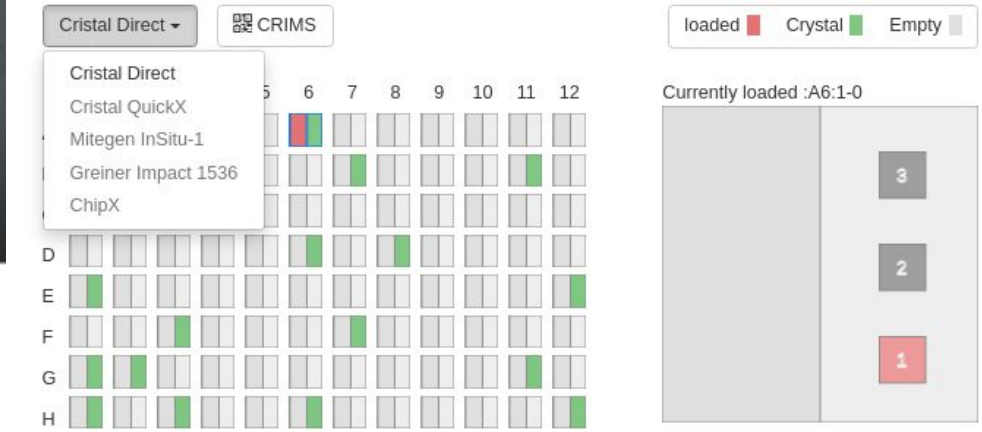


M Oscarsson and JB Florial

IN SITU DATA COLLECTION

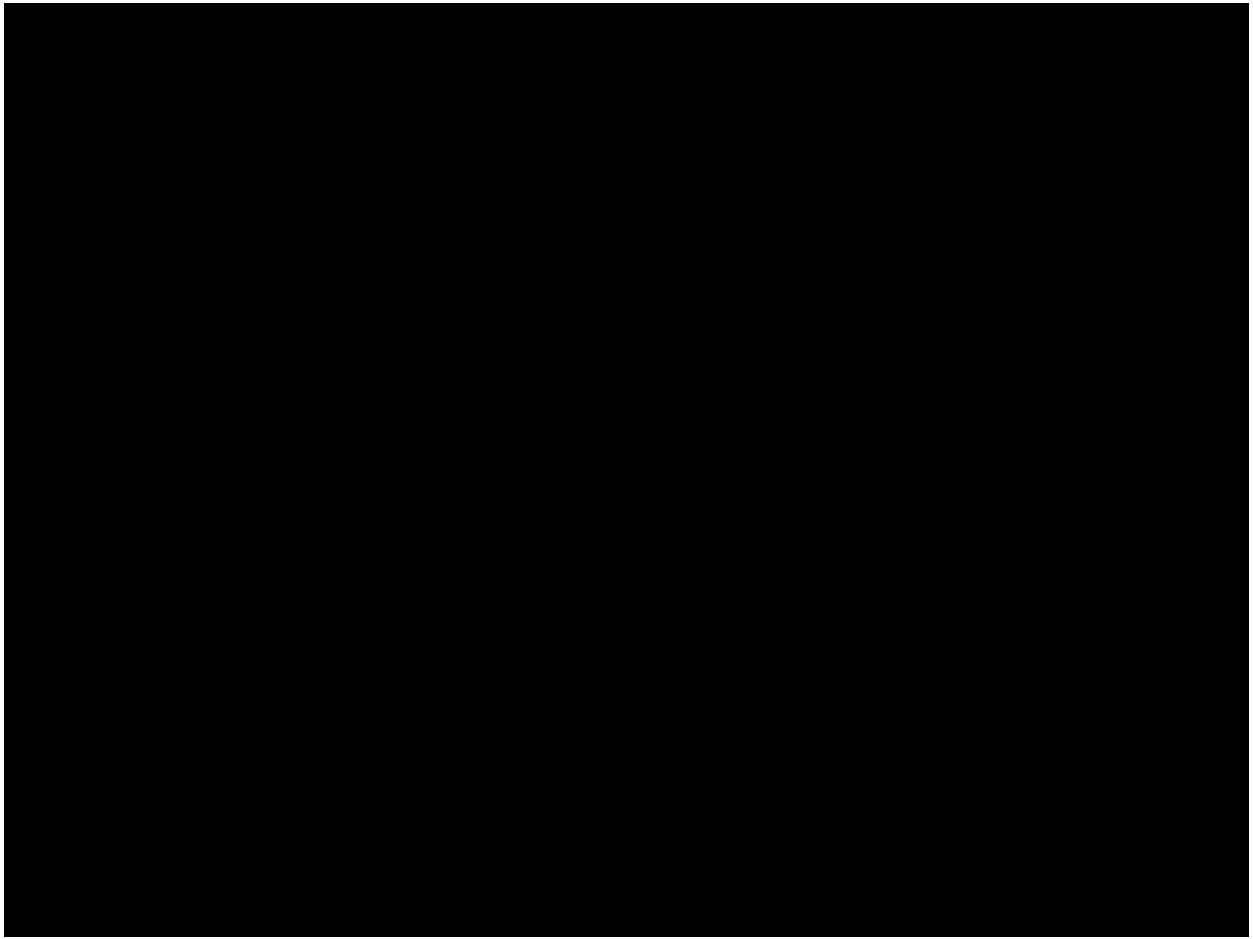


- Experimental workflow within the current implementation :
- Crystal screening:
  - based on known position X-Y CRIMS (synch) (Harvesting plan)
  - Or mesh scan on each drop

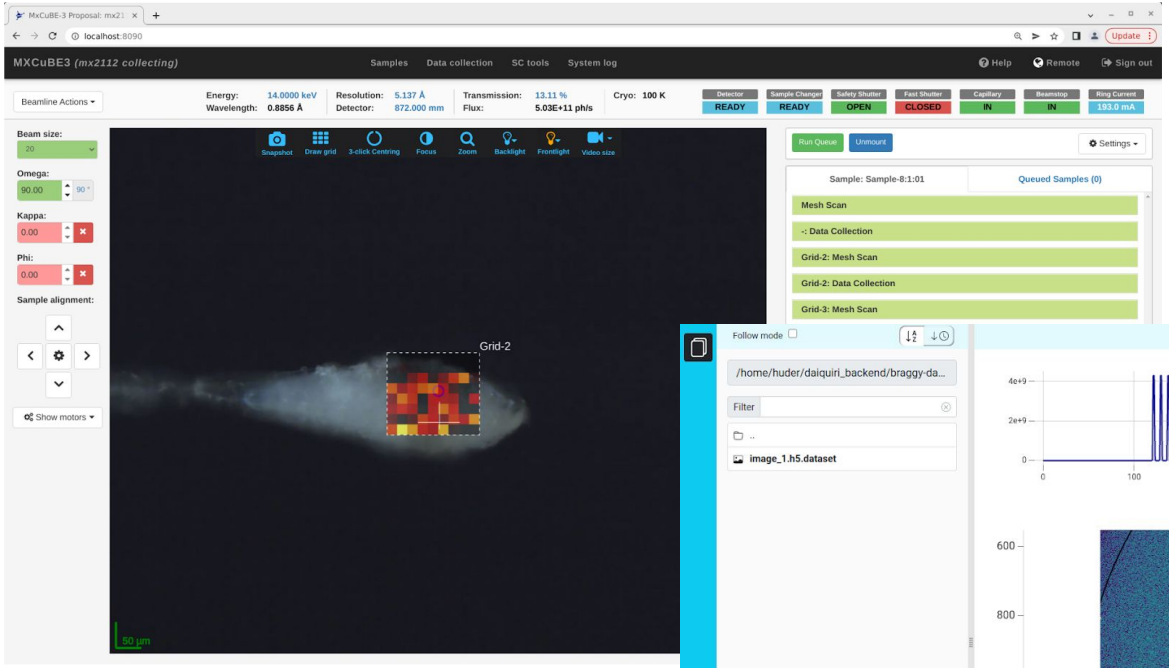


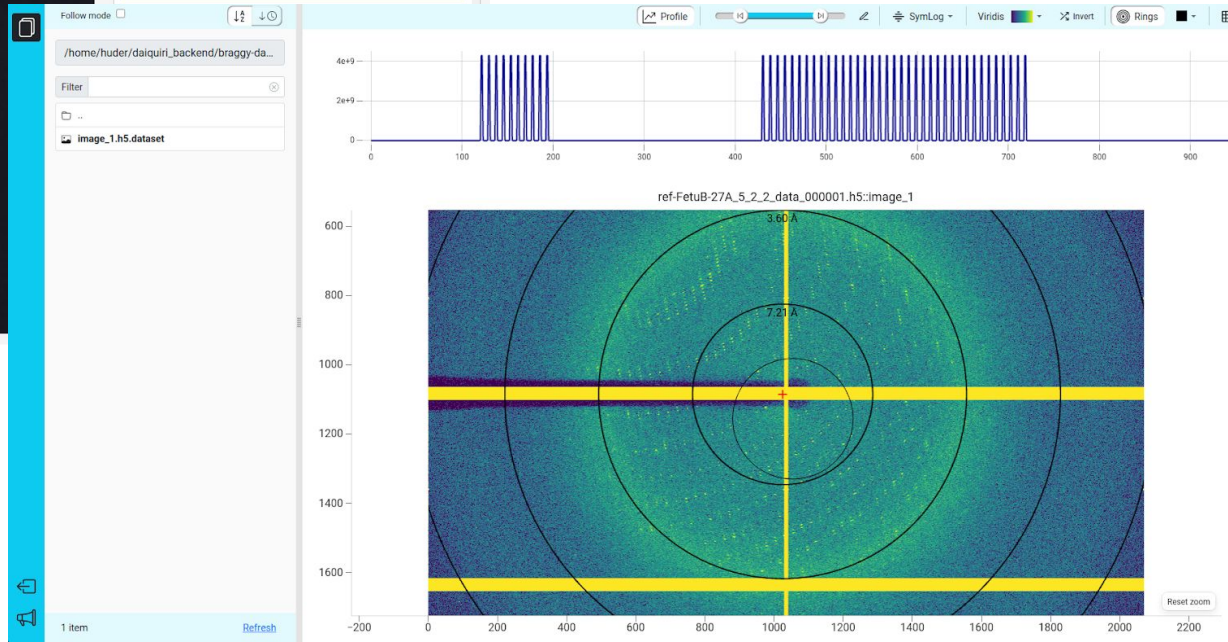
M Oscarsson, J,B Florial, N. Foos, A Beteva

IN SITU DATA COLLECTION



BRAGGY INTERACTIVE MESH

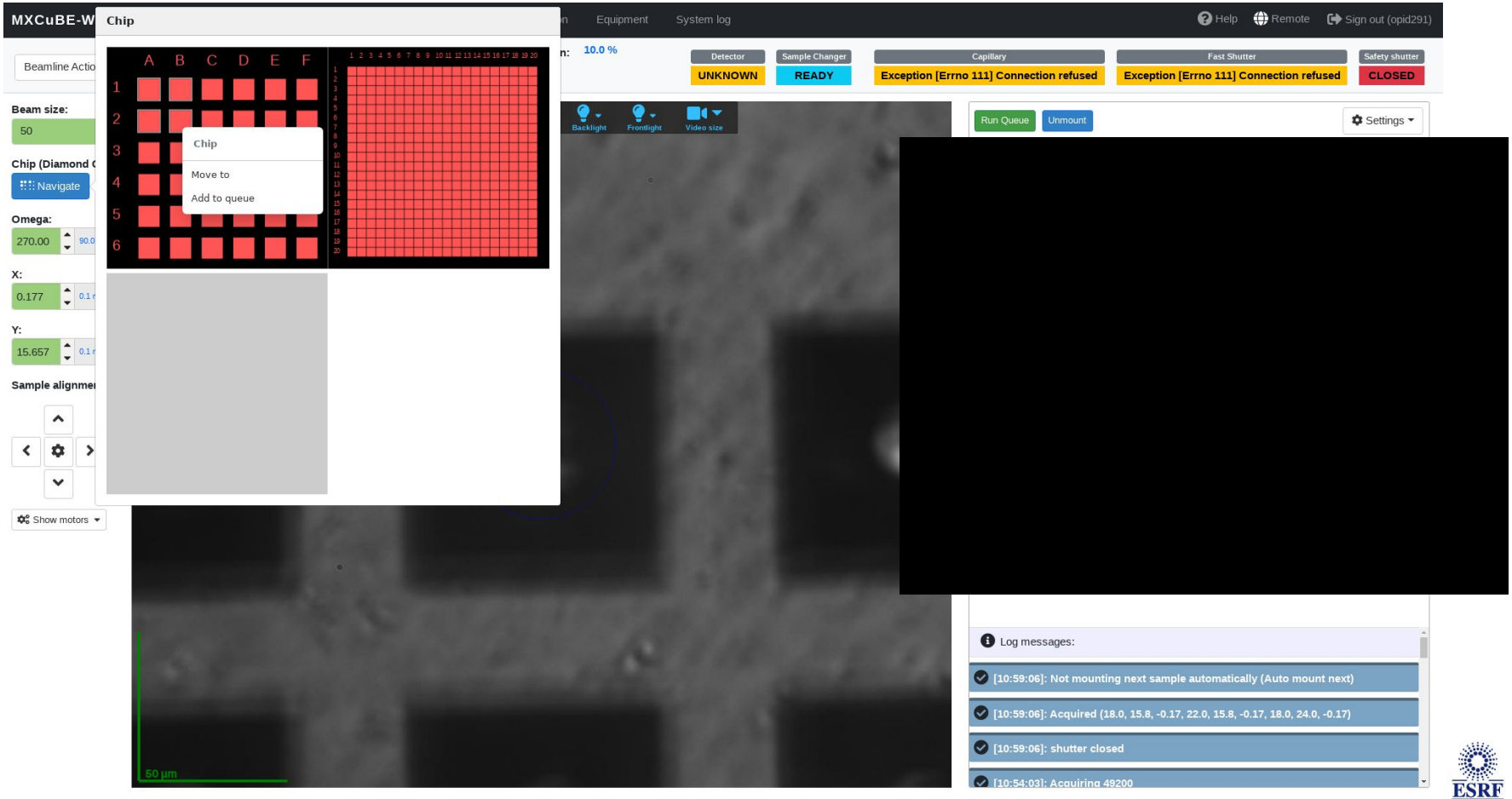




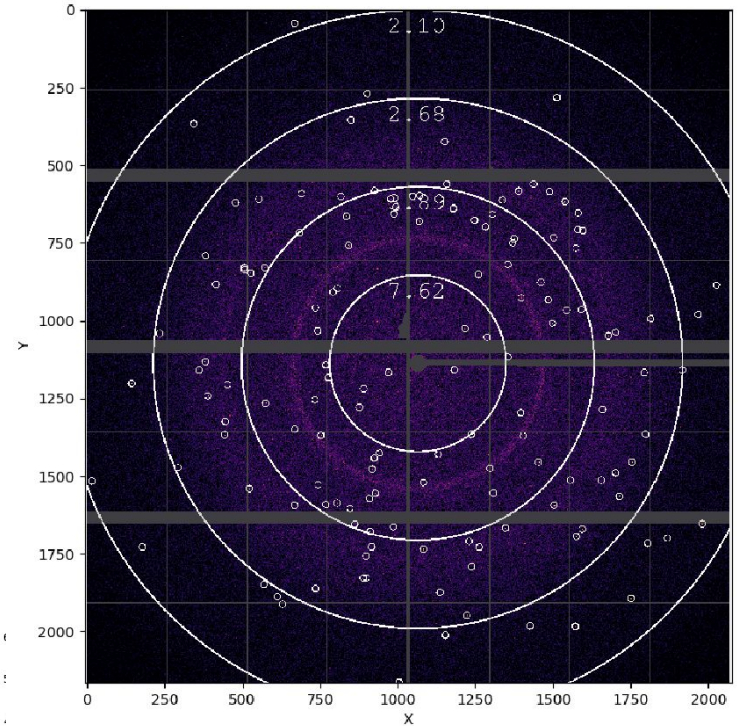
Socket can be sent also to adxv, albula

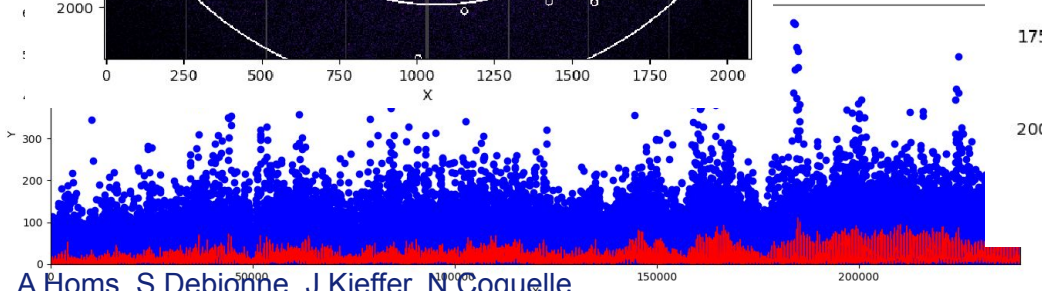
M Oscarsson and A Bocciarelli

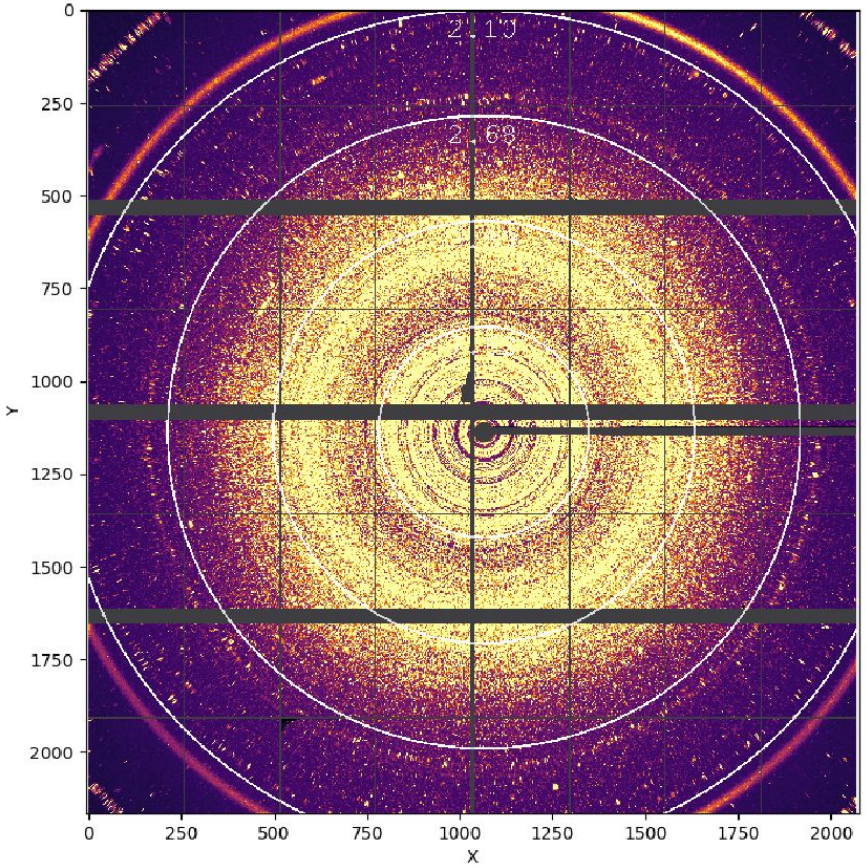
ID29


MXCuBE-W
Chip
Equipment
System log
Help
Remote
Sign out (opid291)
Beamline Actio
10.0 %
Detector
UNKNOWN
Sample Changer
READY
Capillary
Exception [Errno 111] Connection refused
Fast Shutter
Exception [Errno 111] Connection refused
Safety shutter
CLOSED
Beam size:
50
Chip (Diamond
Navigate
Omega:
270.00
X:
0.177
Y:
15.657
Sample alignme
Show motors
A B C D E F
1 2 3 4 5 6
Chip
Move to
Add to queue
Backlight
Frontlight
Video size
Run Queue
Unmount
Settings
50 µm
Log messages:
[10:59:06]: Not mounting next sample automatically (Auto mount next)
[10:59:06]: Acquired (18.0, 15.8, -0.17, 22.0, 15.8, -0.17, 18.0, 24.0, -0.17)
[10:59:06]: shutter closed
[10:54:03]: Acquiring 49200

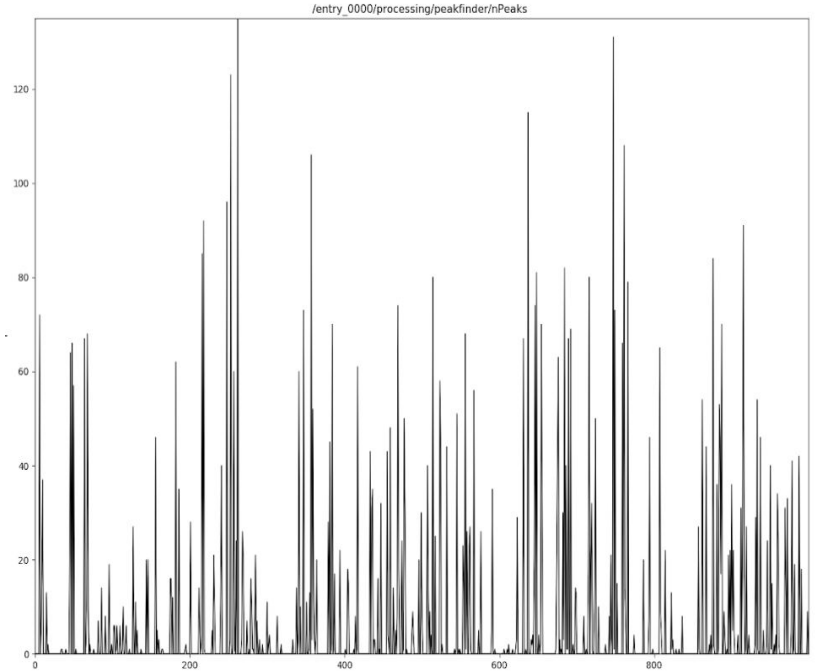
ID29

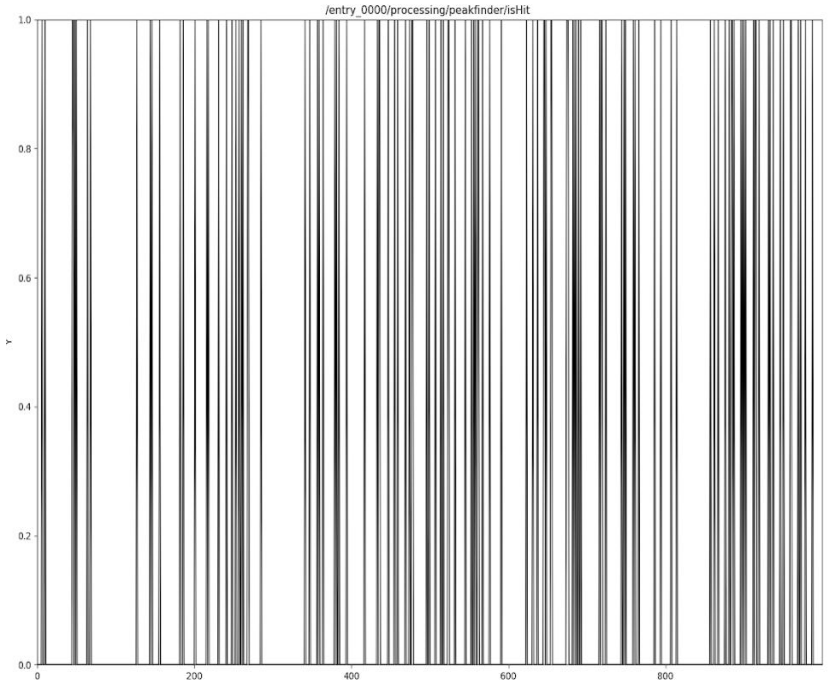






HIT-FINDING IN DAQ SEQUENCE





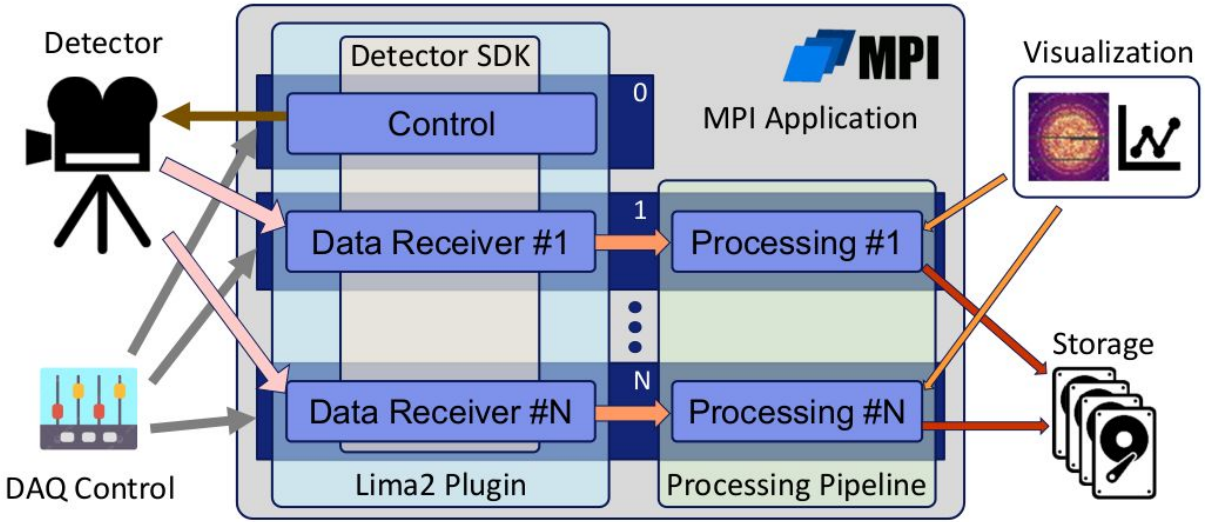
- **Identify** the presence of **diffraction spots** directly in the **DAQ**
- **LImA2** detects spots and flags frames above a certain threshold directly in GPU
  - Possibility for automatic sorting reducing saved data and data bandwidth
  - Algorithm based on pyFAI is the same as in the offline analysis
  - Currently under final commissioning
  - Hits are written and flagged in the hdf5 files directly

A Homs, S Debionne, J Kieffer, N Coquelle

LIMA2

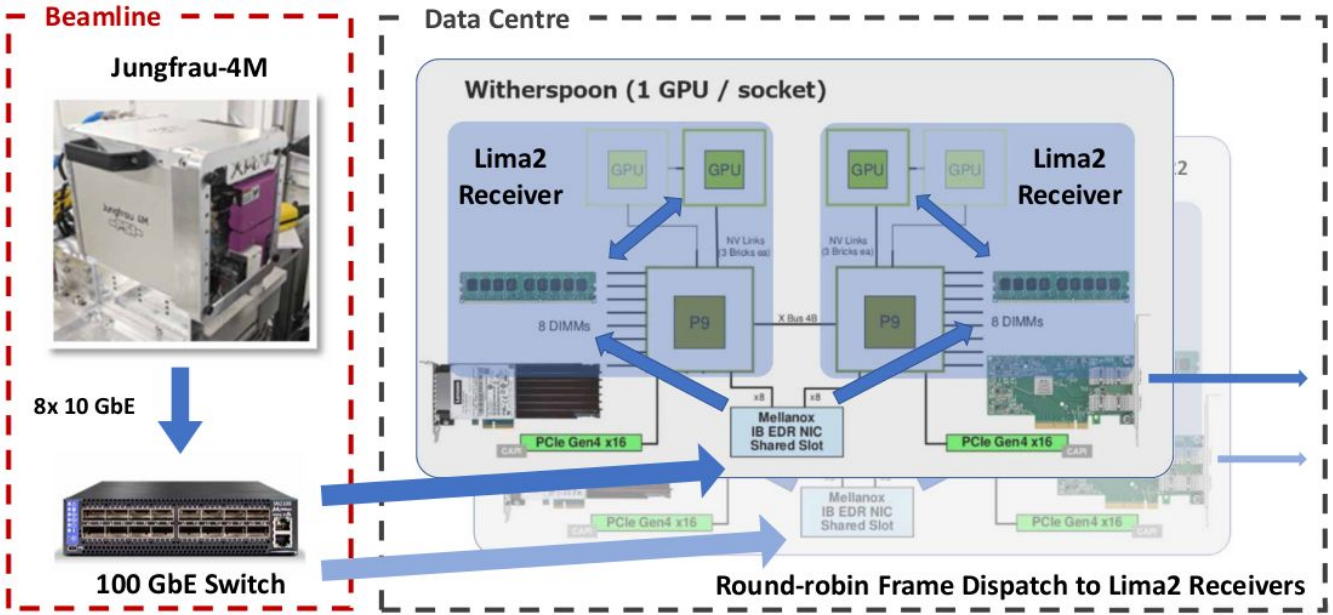
S. Debionne, A. Homs Puron, J. Keiffer, R. Ponsard, L. Claustre, A. Götz, P. Fajardo
European Synchrotron Radiation Facility (ESRF), Grenoble, France

- LImA2: evolution of LImA towards distributed systems (from scratch)
- Goals: scalable DAQ and low latency processing



- C++ library
- Separate DAQ from processing
- Feature extraction and advanced data reduction
- Specific & optimized pipelines

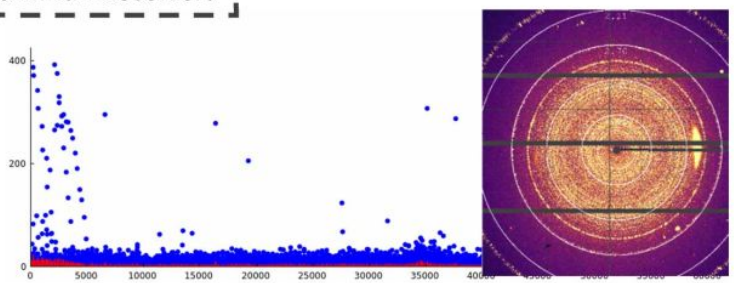
LIMA2



Parallel streams:
- 2x computers
- 2x receivers / computer

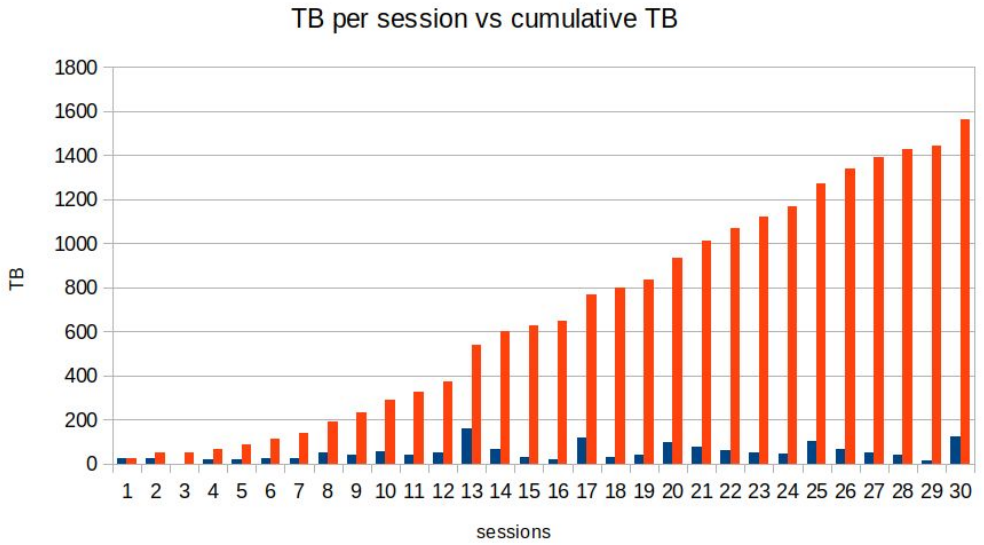
GPU:
- Geometry assembly
- Pedestal/gain correction
- Data sparsification
- Peak finding

- Sparse data: x4-x100 factor reduction
- *Is-hit* information can be used as veto
- In production since January 2023
- Low-latency online visualization
- Continuous processing @ 500 Hz ⇨ 1 kHz



HOW TO DEAL WITH DATA THROUGHPUT

- Migrate to int16 or float16
- Reject frames on the fly
  - Reduce file sizes and increase frame rate
- Off-line image sorting
  - Keep only meaningful frames in the long term



NEXT (SHORT TERM) MILESTONES

- Advance on SSX ID29 specific features
- Develop specific data sorting / pre-analysis
- Braggy visualisation of Jungfrau images
  - Hits display
  - Max Projection
- Deploy MASSIF1 workflows on other beamlines
- Port data collection routines to Bliss
- ICAT integration
- Deploy SSO (and 2FA) and proposal selection