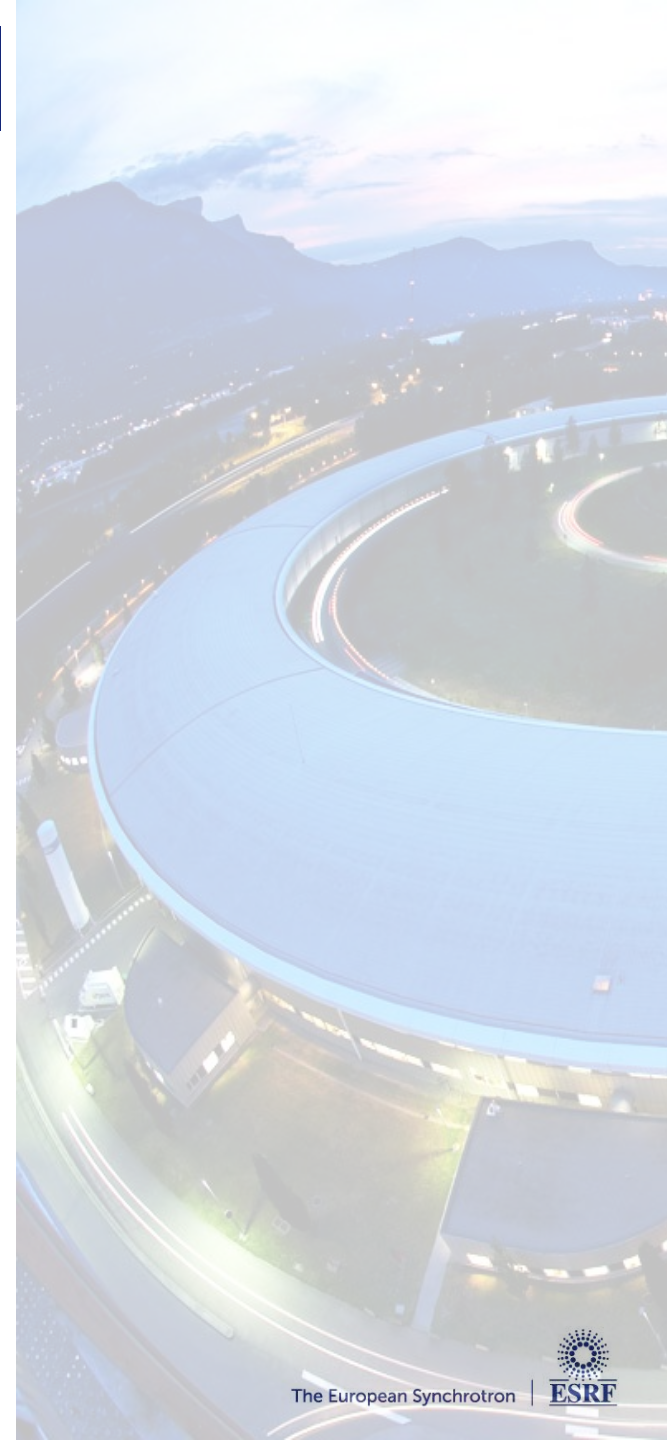




- **News from the developers committee**
- **Feature review**
- **MXCUBE at ESRF**





On behalf of the
developers committee

- As always monthly meetings - minutes can be found at https://mxcube.github.io/mxcube/doc/developers_meetings/index.html

From last MXCuBE meeting discussions on: Configuration - XML to YAML conversion, web-security and deployment, new queue features, unattended data collections

- Code camp on mxcubecore and mxcubeweb development with an introduction to Javascript and React development - October 2023

Talks and minutes available on:

https://mxcube.github.io/mxcube/doc/developers_meetings/index.html

- Code camp on documentation - March 2024

Very nice collaborative effort resulting in:

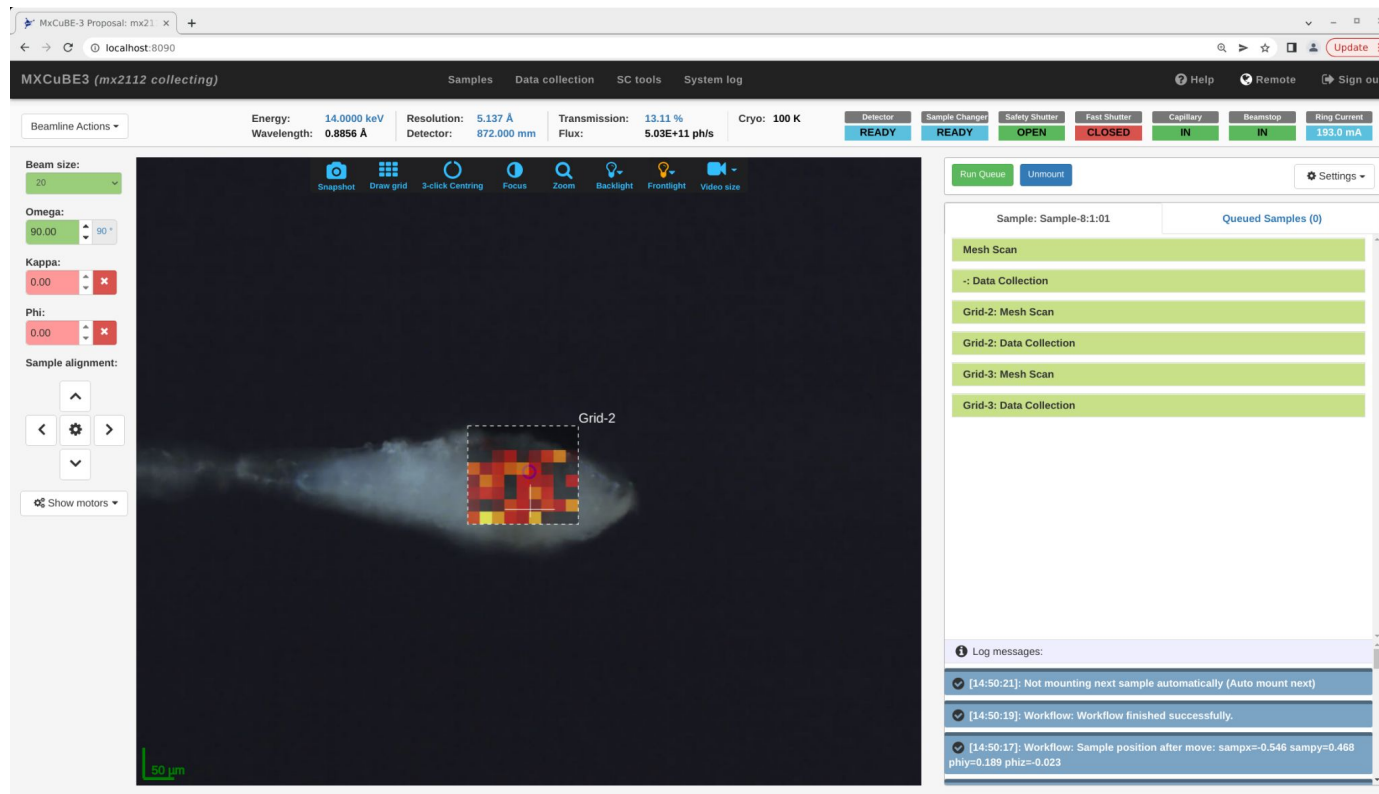
<https://mxcubeweb.readthedocs.io>

<https://mxcubecore.readthedocs.io>

Still in progress and a continuous process !



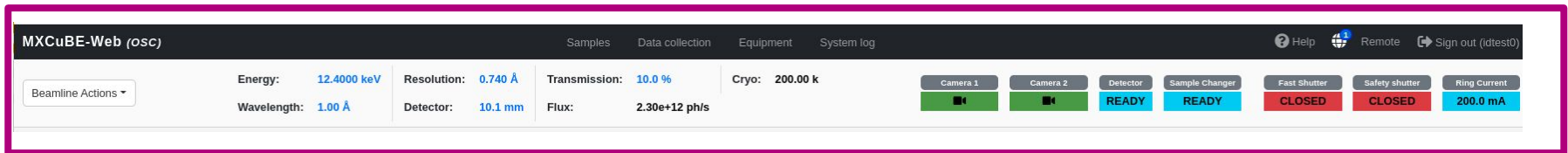
Feature review



Same principle interface on all sites

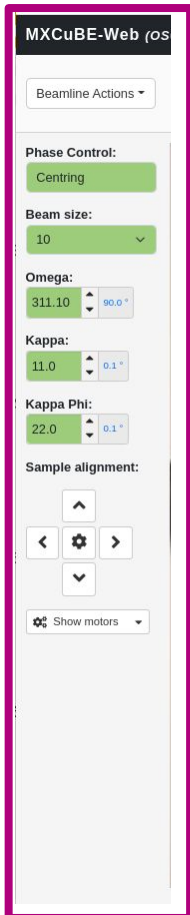
To a certain extent configurable **instrumentation control**, **procedures / methods**

The screenshot displays the MXCuBE-Web (osc) interface. At the top, a navigation bar includes tabs for Samples, Data collection, Equipment (highlighted with a blue box), and System log. Below this, a status bar shows key parameters: Energy (12.4000 keV), Resolution (0.740 Å), Transmission (10.0 %), Cryo (200.00 k), Wavelength (1.00 Å), Detector (10.1 mm), and Flux (2.30e+12 ph/s). A 'Beamline Actions' dropdown is highlighted with a blue box. The main interface is divided into three main sections. On the left, the 'Phase Control' panel is highlighted with a blue box, containing controls for Centring, Beam size (10), Omega (311.10), Kappa (11.0), Kappa Phi (22.0), and Sample alignment. The central area features a large image of a sample, with a context menu open over it. The menu options include 'Go To Beam', 'Measure Distance', 'Draw Grid', 'Data Collection (Limited OSC)', 'Characterisation (1 Image)', 'SSX Chip Collection (Lima1)' (highlighted with a blue box), 'Test Collection', 'GΦL Translational Calibration', 'MXPressE', 'Trouble shooting', and 'Trouble shooting Dialog'. On the right, the 'Run Queue' panel is highlighted with a blue box, showing 'Sample: test - test' and 'Queued Samples (0)'. At the bottom right, a 'Log messages' section displays a message: '[12:29:08]: Mounting sample: test'.



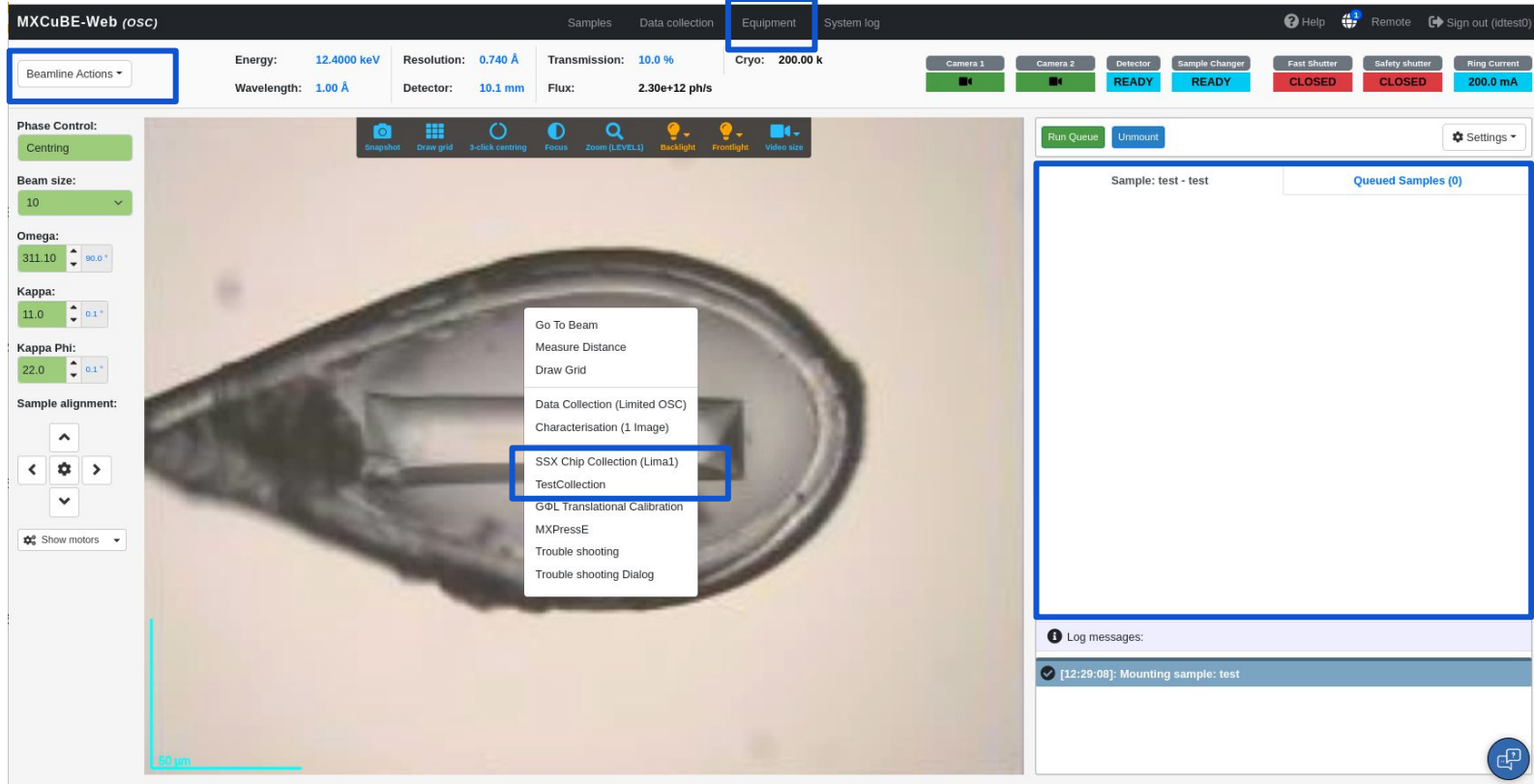
The display of available instrumentation is configurable in ui.yaml

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



```
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: " °"
```

```
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
```



- **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

Equipment view - For less often or temporary instrumentation commands

- For convenience, maintenance and workarounds
- Automatic simple test/maintenance UI for type hinted and “exported” (in .xml file)
- Possible via typehints

MXCuBE-Web (osc)

Samples Data collection Equipment System log Help Remote Sign out (dtest0)

Mockup READY

Content

Refresh Scan all containers

+ Mockup

Power

PowerOn PowerOff Regulation On

Lid

Open Lid Close Lid

Actions

Home Dry Soak

Recovery

Clear Memory Reset Message Back Safe

Abort

Abort

my_fancy_function

my_fancy_function Last result

Speed*

Num Images*

Exp Time*

PhaseEnum*
An enumeration.

Run my_fancy_function

detector READY

diffractometer READY

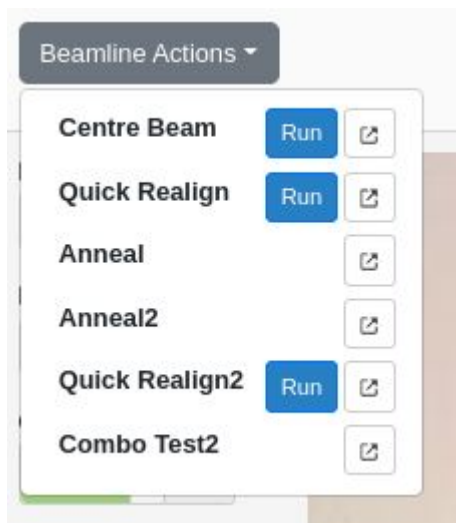
abort my_fancy_function

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.m
    {"type": "controller", "name": "Quick Realign", "command": "HardwareObjects
    {"type": "controller", "name": "Anneal", "command": "HardwareObjects.mockup
    {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMock
    {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMock
    {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMock
  ]
</commands>
</object>
```

The controller commands define the command arguments programmatically via the `CommandObject.add_argument` method

The annotated command uses the method typehints and Pydantic models to define the arguments

Example beamline action - anneal dialog

The screenshot displays the MXCuBE-Web (SSX-CHIP) control interface. At the top, navigation tabs include 'Samples', 'Data collection', 'Equipment', and 'System log'. The top right corner features links for 'Help', 'Remote', and 'Sign out (opid291)'. The main header area shows key parameters: Energy: 12.4000 KeV, Resolution: 1.037 Å, Transmission: 10.0 %, Wavelength: 1.00 Å, Detector: 10.1 mm, and Flux: 0.00e+0 ph/s. Below these are status buttons for Detector (UNKNOWN), Sample Changer (READY), Beamstop (OUT), Capillary (IN), Fast Shutter (CLOSED), Safety shutter (CLOSED), and Ring Current (-1). On the left, a 'Beamline Actions' dropdown menu is open, showing options: 'Centre Beam', 'Quick Realign', 'Anneal', and 'Navigate'. The 'Anneal' option is selected. A central 'Anneal' dialog box is open, containing a 'Time [s]' input field and a 'Run' button. At the bottom right of the dialog is a 'Close window' button. The background interface also shows motor controls for Omega (311.10), Kappa (11.0), and Kappa Phi (22.0), along with a 'Sample alignment' section with directional buttons and a 'Show motors' toggle.

Feature review

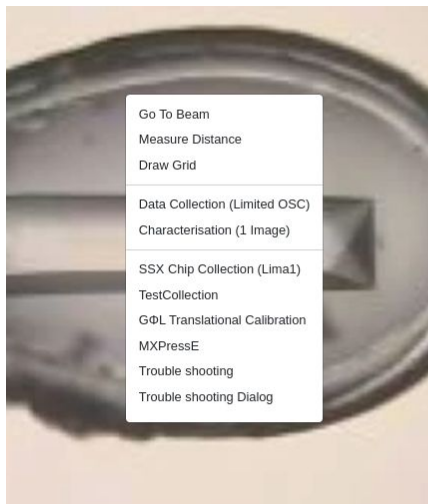
Queue entry / task - For collecting data

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

```
82     legacy_parameters: LegacyParameters
83
84
85     class SsxChipCollectionQueueEntry(BaseQueueEntry):
86         """
87         Defines the behaviour of a data collection.
88         """
89         DATA_MODEL = SsxChipCollectionTaskParameters
90         NAME = "SSXChipCollection"
91         REQUIRES = ["point", "line", "no_shape", "chip", "mesh"]
92
93         # New style queue entry does not take view argument,
94         # adding kwargs for compatability, but they are unused
95         def __init__(self, data: SsxChipCollectionTaskParameters, view=None,
96                     super().__init__(view=view, data_model=TaskNode(data))
97
98
99         def execute(self):
100             super().execute()
```

```
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
```

Model parsed JSONSchema generated and a dialog can be created



Wavelength: 1.00 Å Detector: 10.1 mm Flux: 1.50e+10 ph/s UNKNOWN

Path: /data/id29/inhouse/opid291/20220916/RAW_DATA/Mb/Mb-Mb/

Filename: Mb-Mb_[RUN#]_[IMG#]

Subdirectory: Mb-Mb-Mb/

Prefix: Mb-Mb

Acquisition

Exp Time: 0.02 Align Chip: ☒

Sub Sampling: 4 Take Pedestal: ☒

Default Parameters Run Now Add to Queue

New sample list

MXCuBE-Web (SSX-CHIP)

Samples

Data collection

Equipment

System log

Help

Remote

Sign out (ldtest0)

Get samples from SC

ISPb

Clear sample list

View Mode

Filter :

Filter options

+ Add to Queue

Settings

Collect 2/384

Cell 1			
Puck 1	Puck 2	Puck 3	
<input type="checkbox"/> Sample-1:1:01 1:1:01	<input type="checkbox"/> Sample-1:2:01 1:2:01	<input checked="" type="checkbox"/> Sample-1:3:01 1:3:01 WF X WF X	
<input type="checkbox"/> Sample-1:1:02 1:1:02	<input type="checkbox"/> Sample-1:2:02 1:2:02	<input type="checkbox"/> Sample-1:3:02 1:3:02	
<input type="checkbox"/> Sample-1:1:03 1:1:03	<input type="checkbox"/> Sample-1:2:03 1:2:03	<input type="checkbox"/> Sample-1:3:03 1:3:03	
<input type="checkbox"/> Sample-1:1:04 1:1:04	<input type="checkbox"/> Sample-1:2:04 1:2:04	<input type="checkbox"/> Sample-1:3:04 1:3:04	
<input type="checkbox"/> Sample-1:1:05 1:1:05	<input type="checkbox"/> Sample-1:2:05 1:2:05	<input type="checkbox"/> Sample-1:3:05 1:3:05	
<input type="checkbox"/> Sample-1:1:06 1:1:06	<input type="checkbox"/> Sample-1:2:06 1:2:06	<input type="checkbox"/> Sample-1:3:06 1:3:06	
<input type="checkbox"/> Sample-1:1:07 1:1:07	<input type="checkbox"/> Sample-1:2:07 1:2:07	<input type="checkbox"/> Sample-1:3:07 1:3:07	
<input type="checkbox"/> Sample-1:1:08 1:1:08	<input type="checkbox"/> Sample-1:2:08 1:2:08	<input type="checkbox"/> Sample-1:3:08 1:3:08	
<input type="checkbox"/> Sample-1:1:09 1:1:09	<input type="checkbox"/> Sample-1:2:09 1:2:09	<input type="checkbox"/> Sample-1:3:09 1:3:09	
<input type="checkbox"/> Sample-1:1:10 1:1:10	<input type="checkbox"/> Sample-1:2:10 1:2:10	<input type="checkbox"/> Sample-1:3:10 1:3:10	
<input type="checkbox"/> Sample-1:1:11 1:1:11	<input type="checkbox"/> Sample-1:2:11 1:2:11	<input type="checkbox"/> Sample-1:3:11 1:3:11	
<input type="checkbox"/> Sample-1:1:12 1:1:12	<input type="checkbox"/> Sample-1:2:12 1:2:12	<input type="checkbox"/> Sample-1:3:12 1:3:12	
<input type="checkbox"/> Sample-1:1:13 1:1:13	<input type="checkbox"/> Sample-1:2:13 1:2:13	<input type="checkbox"/> Sample-1:3:13 1:3:13	

Cell 2			
Puck 1	Puck 2	Puck 3	
<input type="checkbox"/> Sample-2:1:01 2:1:01	<input type="checkbox"/> Sample-2:2:01 2:2:01	<input type="checkbox"/> Sample-2:3:01 2:3:01	
<input checked="" type="checkbox"/> Sample-2:1:02 2:1:02 DC X	<input type="checkbox"/> Sample-2:2:02 2:2:02	<input type="checkbox"/> Sample-2:3:02 2:3:02	
<input type="checkbox"/> Sample-2:1:03 2:1:03	<input type="checkbox"/> Sample-2:2:03 2:2:03	<input type="checkbox"/> Sample-2:3:03 2:3:03	
<input type="checkbox"/> Sample-2:1:04 2:1:04	<input type="checkbox"/> Sample-2:2:04 2:2:04	<input type="checkbox"/> Sample-2:3:04 2:3:04	
<input type="checkbox"/> Sample-2:1:05 2:1:05	<input type="checkbox"/> Sample-2:2:05 2:2:05	<input type="checkbox"/> Sample-2:3:05 2:3:05	
<input type="checkbox"/> Sample-2:1:06 2:1:06	<input type="checkbox"/> Sample-2:2:06 2:2:06	<input type="checkbox"/> Sample-2:3:06 2:3:06	
<input type="checkbox"/> Sample-2:1:07 2:1:07	<input type="checkbox"/> Sample-2:2:07 2:2:07	<input type="checkbox"/> Sample-2:3:07 2:3:07	
<input type="checkbox"/> Sample-2:1:08 2:1:08	<input type="checkbox"/> Sample-2:2:08 2:2:08	<input type="checkbox"/> Sample-2:3:08 2:3:08	
<input type="checkbox"/> Sample-2:1:09 2:1:09	<input type="checkbox"/> Sample-2:2:09 2:2:09	<input type="checkbox"/> Sample-2:3:09 2:3:09	
<input type="checkbox"/> Sample-2:1:10 2:1:10	<input type="checkbox"/> Sample-2:2:10 2:2:10	<input type="checkbox"/> Sample-2:3:10 2:3:10	
<input type="checkbox"/> Sample-2:1:11 2:1:11	<input type="checkbox"/> Sample-2:2:11 2:2:11	<input type="checkbox"/> Sample-2:3:11 2:3:11	
<input type="checkbox"/> Sample-2:1:12 2:1:12	<input type="checkbox"/> Sample-2:2:12 2:2:12	<input type="checkbox"/> Sample-2:3:12 2:3:12	
<input type="checkbox"/> Sample-2:1:13 2:1:13	<input type="checkbox"/> Sample-2:2:13 2:2:13	<input type="checkbox"/> Sample-2:3:13 2:3:13	

New sample list

Get samples from SC ▾ ISPyB → Clear sample list View Mode ▾ Filter : ▾ + Add to Queue ▾ Settings ▾ Collect 17/368 >

Cell 1 Selected

Cell 1 ▢ ≡

Puck 1	Puck 2	Puck 3
<input checked="" type="checkbox"/> Sample-1:1:01 1:1:01 1	<input type="checkbox"/> Sample-1:2:01 1:2:01	<input type="checkbox"/> Sample-1:3:01 1:3:01
<input checked="" type="checkbox"/> Sample-1:1:02 1:1:02 2	<input type="checkbox"/> Sample-1:2:02 1:2:02	<input type="checkbox"/> Sample-1:3:02 1:3:02
<input checked="" type="checkbox"/> Sample-1:1:03 1:1:03 3	<input type="checkbox"/> Sample-1:2:03 1:2:03	<input type="checkbox"/> Sample-1:3:03 1:3:03
<input checked="" type="checkbox"/> Sample-1:1:04 1:1:04 4	<input type="checkbox"/> Sample-1:2:04 1:2:04	<input type="checkbox"/> Sample-1:3:04 1:3:04
<input checked="" type="checkbox"/> Sample-1:1:05 1:1:05 5	<input type="checkbox"/> Sample-1:2:05 1:2:05	<input type="checkbox"/> Sample-1:3:05 1:3:05
<input checked="" type="checkbox"/> Sample-1:1:06 1:1:06 6	<input type="checkbox"/> Sample-1:2:06 1:2:06	<input type="checkbox"/> Sample-1:3:06 1:3:06
<input checked="" type="checkbox"/> Sample-1:1:07 1:1:07 7	<input type="checkbox"/> Sample-1:2:07 1:2:07	<input type="checkbox"/> Sample-1:3:07 1:3:07
<input checked="" type="checkbox"/> Sample-1:1:08 1:1:08 8	<input type="checkbox"/> Sample-1:2:08 1:2:08	<input type="checkbox"/> Sample-1:3:08 1:3:08
<input checked="" type="checkbox"/> Sample-1:1:09 1:1:09 9	<input type="checkbox"/> Sample-1:2:09 1:2:09	<input type="checkbox"/> Sample-1:3:09 1:3:09
<input checked="" type="checkbox"/> Sample-1:1:10 1:1:10 10	<input type="checkbox"/> Sample-1:2:10 1:2:10	<input type="checkbox"/> Sample-1:3:10 1:3:10
<input checked="" type="checkbox"/> Sample-1:1:11 1:1:11 11	<input type="checkbox"/> Sample-1:2:11 1:2:11	<input type="checkbox"/> Sample-1:3:11 1:3:11
<input checked="" type="checkbox"/> Sample-1:1:12 1:1:12 12	<input type="checkbox"/> Sample-1:2:12 1:2:12	<input type="checkbox"/> Sample-1:3:12 1:3:12
<input checked="" type="checkbox"/> Sample-1:1:13 1:1:13 13	<input type="checkbox"/> Sample-1:2:13 1:2:13	<input type="checkbox"/> Sample-1:3:13 1:3:13

Thanks JB



MXCUBE at ESRF

- ID23-1, ID23-2, ID30B and ID29 on **mxcube-web-4.72.0+esrf.0516** and **mxcube-core-1.104.0+esrf.0516** (ID30A1 and ID30A3 are being updated)
- We try to rebase on upstream and deploy roughly every two weeks - this would be helped by better test coverage :)
- SSO with two factor authentication
- ICAT integration ongoing

Single sign on with new proposal selection interface

The screenshot shows the 'Select a session' dialog box with the 'Scheduled' tab selected. It lists four sessions:

Session ID	Session Name	Start Date	End Date	Shortcuts
OA6	PSI- Novartis through Expose	20/02/2024 09:30:00	23/02/2024 08:00:00	Portal A-Form Logbook
OA5	PSI-Roche through Expose	20/02/2024 09:30:00	23/02/2024 08:00:00	Portal A-Form Logbook
OA4	PSI-Boehringer Ingelheim Vienna through Expose	20/02/2024 09:30:00	23/02/2024 08:00:00	Portal A-Form Logbook
OA3	PSI-Boehringer Ingelheim Biberach through Expose			

Buttons at the bottom: Cancel, Select Proposal.

The screenshot shows the 'Select a session' dialog box with the 'Scheduled' tab selected. It lists three sessions:

Session ID	Session Name	Start Date	End Date	Beamline	Shortcuts
IX98	Expose GmbH for Biogen	17/02/2024 17:00:00	18/02/2024 01:00:00	ID23-1	Portal A-Form Logbook
FX29	Contract Crystallography (MX)	22/02/2024 09:30:00	22/02/2024 17:00:00	ID30A-1	Portal A-Form Logbook
MX2503	PROTEINS RELATED TO PATHOGENESIS OF DISEASES, VIRAL PROTEINS, CELL DIVISION, SIGNALLING AND CHROMATIN PROCESSES	17/02/2024 09:30:00	18/02/2024 01:00:00	ID30A-1	Portal A-Form Logbook

Buttons at the bottom: Cancel, Select Proposal.

Currently being validated - to be deployed within shortly

Thanks Alejandro !



- Automation features developed on MASSIF1 now available everywhere
- Automation speed up - we are now up to 16 samples per hour (depending on workflow)
- Continued SSX development
 - Chip
 - Foil
 - Injector
 - *Laser triggered*

The screenshot displays the MXCUBE software interface. At the top, a status bar shows 'Wavelength: 1.00 Å', 'Detector: 10.1 mm', and 'Flux: 1.50e+10 ph/s'. A 'Snapshots' icon is visible on the left. The main window is a configuration dialog for a sample run. It includes fields for 'Path' (set to '/data/id29/inhouse/opid291/20220916/RAW_DATA/Mb/Mb-Mb/'), 'Filename' (set to 'Mb-Mb_[RUN#]_[IMG#]'), 'Subdirectory' (set to 'Mb/Mb-Mb/'), and 'Prefix' (set to 'Mb-Mb'). Below these fields is an 'Acquisition' section with 'Exp Time' set to '0.02' and 'Sub Sampling' set to '4'. There are two checkboxes: 'Align Chip' (checked) and 'Take Pedestal' (checked). At the bottom of the dialog are buttons for 'Default Parameters', 'Run Now', and 'Add to Queue'. The background shows a queue of samples with labels like 'UNKNOWN', 'Sant', 'SSXFoilC', 'SSXFoilC', 'SSXInject', 'SSXInject', 'SSXInject', 'SSXInject', and 'SSXInject'.

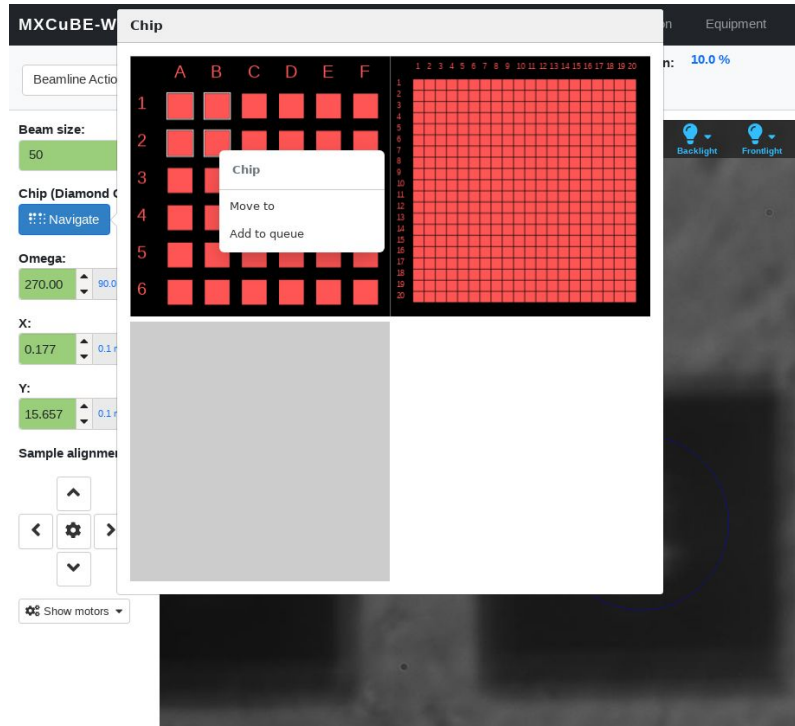
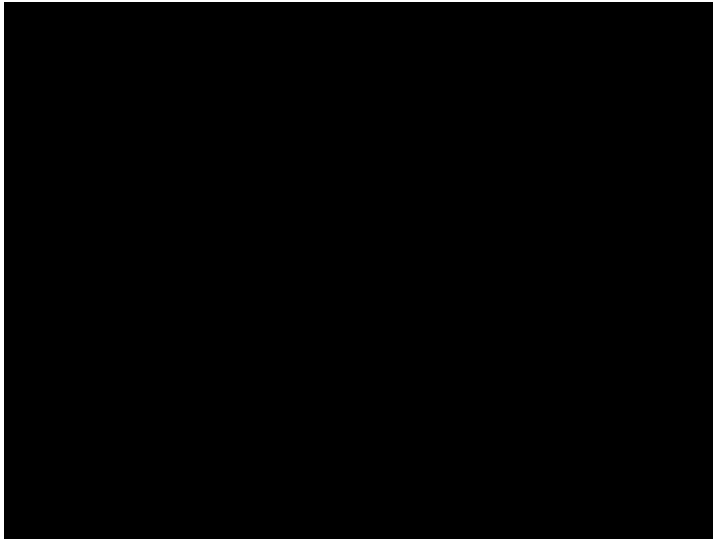
Future perspectives

- Continue SSX development
- Continue development on new queue functionality
- Continue development of automation
- Continue ICAT integration
- Continue work on AbstractProcessing - been on hold for sometime
- Migrating from XML to YAML
- Deploy video stream solution for hutch videos
- Move to TypeScript ?
- Increase testing both backend and e2e
- Cleanup REST API and possibly exchange spectree for FlaskOpenAPI3 ?

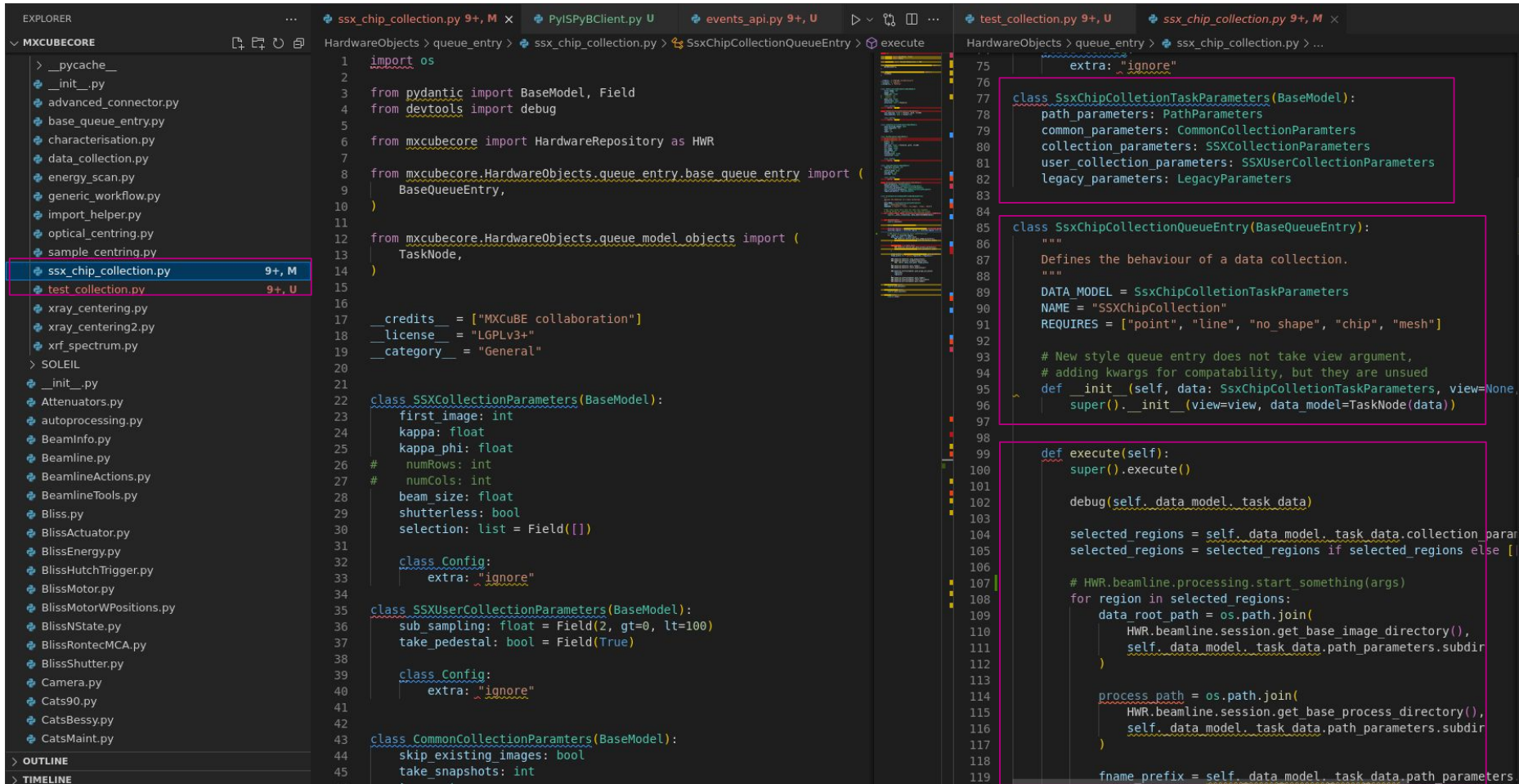
Thank you for your attention







Example - New style queue entry



The screenshot displays a code editor with three open files: `ssx_chip_collection.py`, `PyISPyBClient.py`, and `events_api.py`. The `ssx_chip_collection.py` file is the primary focus, showing a new style queue entry implementation. The code is organized into several classes and methods, with line numbers visible on the left. The `SSXCollectionParameters` class defines parameters for data collection, including `first_image`, `kappa`, `kappa_phi`, `numRows`, `numCols`, `beam_size`, `shutterless`, and `selection`. The `SSXUserCollectionParameters` class defines user-specific parameters like `sub_sampling` and `take_pedestal`. The `CommonCollectionParameters` class defines common parameters like `skip_existing_images` and `take_snapshots`. The `SsxChipCollectionTaskParameters` class defines task-specific parameters like `path_parameters`, `common_parameters`, `collection_parameters`, `user_collection_parameters`, and `legacy_parameters`. The `SsxChipCollectionQueueEntry` class defines the behavior of a data collection, including the `execute` method. The `execute` method is highlighted with a pink box, showing the logic for selecting regions, processing data, and saving files. The `test_collection.py` file is also open, showing a `test_collection` function that uses the `SsxChipCollectionQueueEntry` class.

```
1 import os
2
3 from pydantic import BaseModel, Field
4 from devtools import debug
5
6 from mxcube_core import HardwareRepository as HWR
7
8 from mxcube_core.HardwareObjects.queue_entry.base_queue_entry import (
9     BaseQueueEntry,
10 )
11
12 from mxcube_core.HardwareObjects.queue_model.objects import (
13     TaskNode,
14 )
15
16
17 _credits_ = ["MXCuBE collaboration"]
18 _license_ = "LGPLV3+"
19 _category_ = "General"
20
21
22 class SSXCollectionParameters(BaseModel):
23     first_image: int
24     kappa: float
25     kappa_phi: float
26     # numRows: int
27     # numCols: int
28     beam_size: float
29     shutterless: bool
30     selection: list = Field([])
31
32     class Config:
33         extra: "ignore"
34
35 class SSXUserCollectionParameters(BaseModel):
36     sub_sampling: float = Field(2, gt=0, lt=100)
37     take_pedestal: bool = Field(True)
38
39     class Config:
40         extra: "ignore"
41
42 class CommonCollectionParameters(BaseModel):
43     skip_existing_images: bool
44     take_snapshots: int
```

Example UI

MXCuBE-Web (SSX-CHIP) Samples Data collection Equipment System log ? Help Remote Sign out (opid291)

Energy: 12.4000 KeV Resolution: ~ Å Transmission: 10.0 %
Wavelength: 1.00 Å Detector: 10.1 mm Flux: 1.50e+10 ph/s

Detector: UNKNOWN Sample Changer: READY Capillary: UNKNOWN Fast Shutter: CLOSED Safety shutter: CLOSED

Beamline Actions ▾

Beam size: 50 ▾

Chip (Diamond Chip):
Navigate

Omega: 359.90 90.0°

X: 0.000 0.1 mm

Y: -49.900 0.1 mm

Sample alignment:
Show motors ▾

50 µm

Path: /data/id29/inhouse/opid291/20220916/RAW_DATA/Mb/Mb-Mb/
Filename: Mb-Mb_[RUN#]_[IMG#]
Subdirectory: Mb/Mb-Mb/
Prefix: Mb-Mb

Acquisition

Exp Time: 0.02 Align Chip: ☒
Sub Sampling: 4 Take Pedestal: ☒

Default Parameters Run Now Add to Queue

Sample: Mb - Mb Queued Samples (0)

SSXFoilCollection
SSXFoilCollection
SSXInjectorCollection
SSXInjectorCollection
SSXInjectorCollection
SSXInjectorCollection

Log messages:
✓ [10:15:35]: Opening OH2 safety shutter
✓ [10:15:35]: Not mounting next sample automatically (Auto mount next)
✓ [10:15:29]: Acquired 1000 images