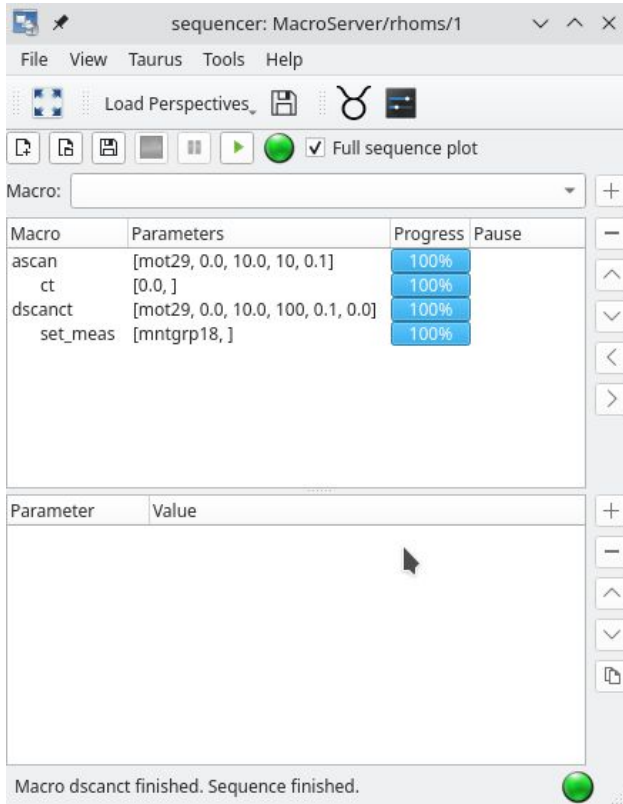


Complex experiment applications at ALBA

Jordi Aguilar
Roberto Homs
Albert Ollé
Zbigniew Reszela
Oriol Vallcorba
Steven Wohl

on behalf of
ALBA Synchrotron
Controls Section

Sardana sequencer



- Easy to use hooks
- Easy to Start/Pause/Restart/Stop
- Easy to save
- Easy to check progress status
- Load from text file (.txt), does not work hooks and params repeats, XML file support them but more complex to write.
- Do not possible to do loops, macro repeat is not adapted (feature/bug)
- Do not possible to do logic blocks (if/else)
- Do not possible to validate parameters (motor limits, valid integration time, ...)
- Do not possible to catch exceptions and recover from fails

BL22 CLAEISS Experiment UI

CLAESS Experiment Sequencer*

File Samples Help

Experiment Folder /home/rhoms/tmp
 Experiment Name 10ke27ke
 Temperature Control Liquid N2

Time (H:M:S): 01:57:38

Sample Holder

Central Position

X 0.00
 Z 4.00

Samples

Pd
 Ru
 Sr
 Nb
 Zr
 Mo
 Sample1

Temperatures (K)

T	Repeats
1 298.1	1
2 180	1
3 234	1

Low to High High to Low

Advanced configurations

RCS

☒ Check incoming intensity

RCS parameters

oh_dcm_xtal2_pitch 1000.00
 energy 15000.00

☐ Moco ON

When

☐ Per each Experiment
☐ Per each Temperature
☒ Per each Sample
☐ Per each Measurement

Experiment Repetitions 1

Measurement

Sample	Type	Mode	Element	Edge/Line	Expert	Temperatures	Repeats	kmax	spp	fluo_x2	slits_hgap	Positions (x, z)
1 Pd	XAS	Transmission	Pd	K	False	[180.0, 298.1]	1	18.0	0.08	100.0	18.0	[[0.0, 0.0]]
2 Ru	XAS	Fluorescence	Ru	K	False	[180.0, 298.1]	1	18.0	0.02	100.0	18.0	[[0.0, 0.0]]
3 Sr	XAS	Fluorescence	Sr	K	False	[180.0, 298.1]	1	18.0	0.1	100.0	18.0	[[0.0, 0.0]]
4 Nb	XAS	Transmission	Nb	K	False	[180.0, 298.1]	1	18.0	0.1	100.0	18.0	[[0.0, 0.0]]
5 Zr	XAS	Fluorescence	Zr	K	False	[180.0, 298.1]	1	18.0	0.2	100.0	18.0	[[0.0, 0.0]]
6 Mo	XAS	Transmission	Mo	K	False	[180.0, 298.1]	1	18.0	0.04	100.0	18.0	[[0.0, 0.0]]
7 Sample1	XAS	Transmission	Ir	L1	False	[234.0, 298.1]	4	8.0	0.2	100.0	18.0	[[6.49, -6.48]]
8 Sample1	XES	Emission	Cu	Ka1	False	[298.1]	1	No applied	0.2	100.0	18.0	[[6.49, -6.48]]

Generate Sequence

Initial requirements:

Easy for external user

Robust

Protections

Recover from fails

Repetitions

Automatic configuration

Temperature Control

Time estimation

Log files

Simulation mode

Work for 90% of proposals

Sardana python 2.7

GUI python 3.9 pyqt=5.15

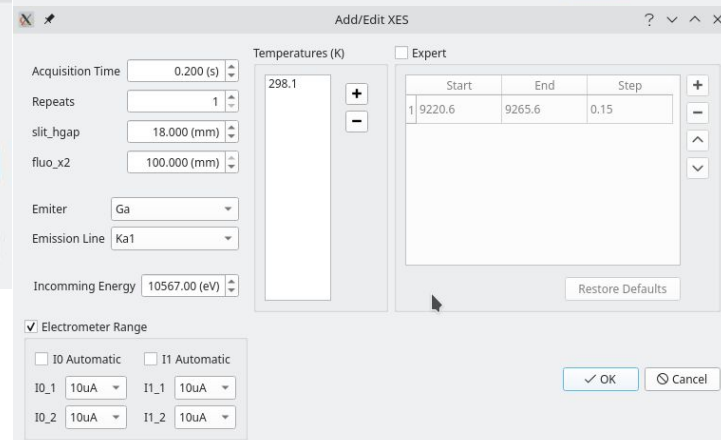
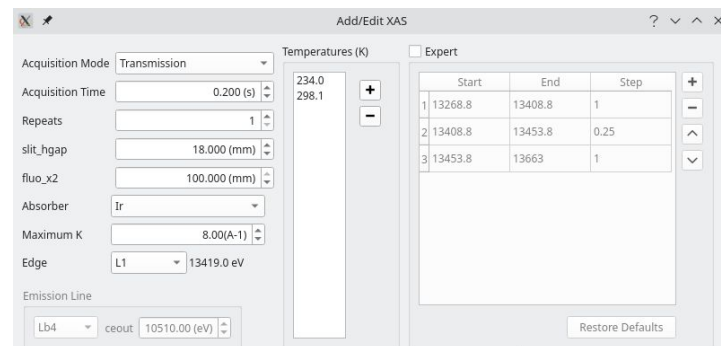
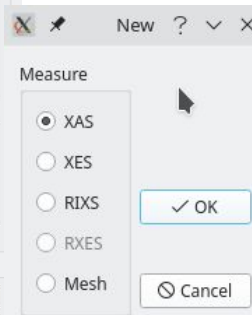
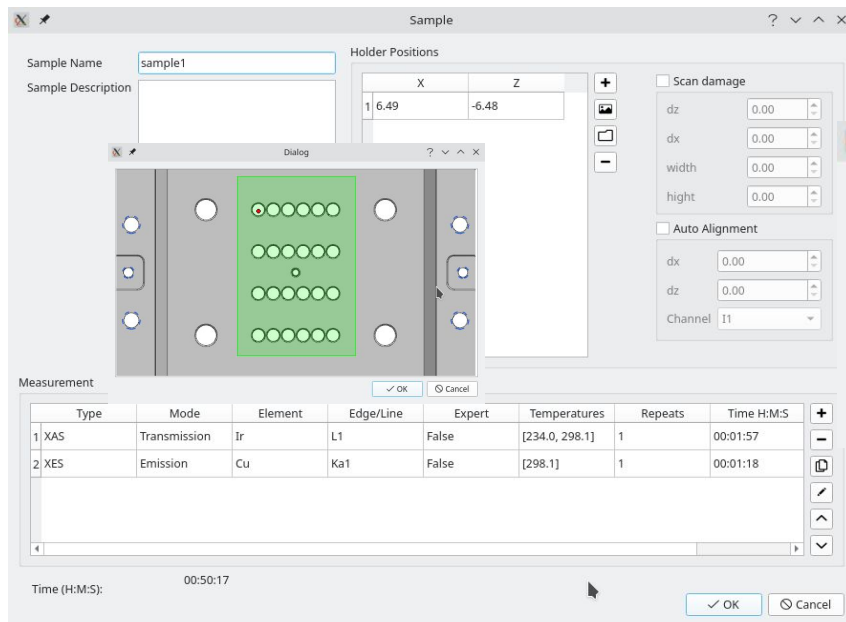
BL22 CLAEISS Experiment UI

Sample position protection (green part)

Measure type selection

Automatic specific configuration, allow Expert mode

Electrometer automatic configuration



BL22 CLAESS Experiment UI

File Samples Help

Experiment Folder /home/rhoms/tmp
Experiment Name 10ke27ke
Temperature Control Liquid N2

Time (H:M:S) 01:57:38

Sample Holder

Samples

Temperatures (K)

T	Repeats
1 298.1	1
2 180	1
3 234	1

Advanced configurations

RCS

☒ Check incoming intensity

RCS parameters

oh_dcm_xtal2_pitch 1000.00
15000.00

When

☐ Per each Experiment
☐ Per each Temperature
☒ Per each Sample
☐ Per each Measurement

Sequence generated

Sequence Saved

The sequence was saved. You can run now the macro from spock:
expguimacro /home/rhoms/tmp/10ke27ke.yaml

OK

Low to High High to Low

XES

Experiment Repetitions 1

Measurement

Sample	Type	Mode	Element	Edge/Line	Expert	Temperatures	Repeats	kmax	spp	fluo_x2	slits_hgap	Positions (x, z)
1 Pd	XAS	Transmission	Pd	K	False	[180.0, 298.1]	1	18.0	0.08	100.0	18.0	[[0.0, 0.0]]
2 Ru	XAS	Fluorescence	Ru	K	False	[180.0, 298.1]	1	18.0	0.02	100.0	18.0	[[0.0, 0.0]]
3 Sr	XAS	Fluorescence	Sr	K	False	[180.0, 298.1]	1	18.0	0.1	100.0	18.0	[[0.0, 0.0]]
4 Nb	XAS	Transmission	Nb	K	False	[180.0, 298.1]	1	18.0	0.1	100.0	18.0	[[0.0, 0.0]]
5 Zr	XAS	Fluorescence	Zr	K	False	[180.0, 298.1]	1	18.0	0.2	100.0	18.0	[[0.0, 0.0]]
6 Mo	XAS	Transmission	Mo	K	False	[180.0, 298.1]	1	18.0	0.04	100.0	18.0	[[0.0, 0.0]]
7 Sample1	XAS	Transmission	Ir	L1	False	[234.0, 298.1]	4	8.0	0.2	100.0	18.0	[[6.49, -6.48]]
8 Sample1	XES	Emission	Cu	Ka1	False	[298.1]	1	No applied	0.2	100.0	18.0	[[6.49, -6.48]]

Generate Sequence



10ke27ke.yaml — KWrite

File Edit Selection View Go Tools

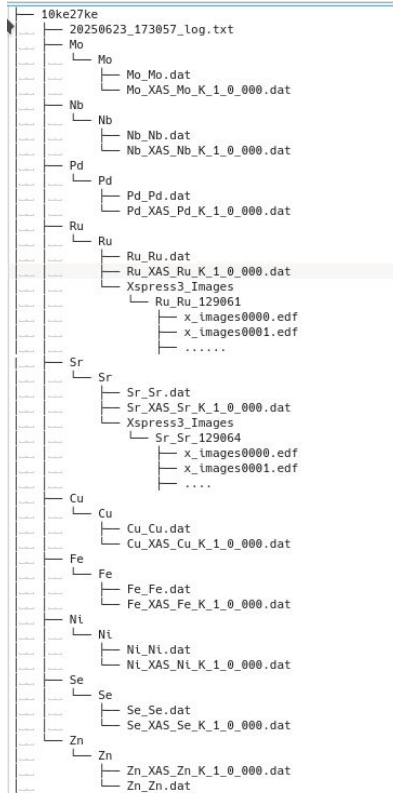
New Open Save

```
experiment_name: 10ke27ke
fit_beam: true
fit_beam_params:
  energy: 15000.0
  method: RCS
  when: PerSample
  xtal2_pitch: 1000.0
loop:
- runs: 1
  samples:
  - auto_align:
    channel: I1
    dx: 0
    dz: 0
    use: false
  measures:
  - acq_time: 0.08
    ceout: 0
    edge: K
    element: Pd
    em:
      i01: 10uA
      i02: 10uA
      i0_auto: false
      i11: 10uA
      i12: 10uA
      i1_auto: false
      use: false
      fluo_x2: 100.0
      mode: Transmission
      ranges:
```

119:15 INSERT en_US Soft Tabs: 4 UTF-8 YAML

BL22 CLAEISS Experiment UI

```
def run(self, filename, run, wait_fe, force_qExafs):
    self.demo = not run
    self._exp_data = None
    self._force_qExafs = force_qExafs
    self._interrupt = False
    self.log_file = None
    try:
        if self.demo:
            self.execMacro = self.infd
        self._exp_data = None
        self.execMacro('blreconfig')
        if wait_fe:
            self.execMacro('blshopen')
        self._run(filename, wait_fe)
    except KeyboardInterrupt:
        self._interrupt = True
        raise
    except Exception as e:
        self.error(msg: 'Exception %s', *args: e, exc_info=True)
    finally:
        if self._exp_data is not None:
            self._save_env()
        if self._interrupt:
            self.error('Macro aborted. Run blreconfig!')
        else:
            self.execMacro('blreconfig')
        if self.log_file is not None:
            for handler in self.log_file.handlers:
                handler.flush()
            self.log_file.removeHandler(handler)
            del handler
```



Sardana TODOs / DONE

Use environment for state saving

(use deepcopy)

Implement abort/stop propagation on
gscan

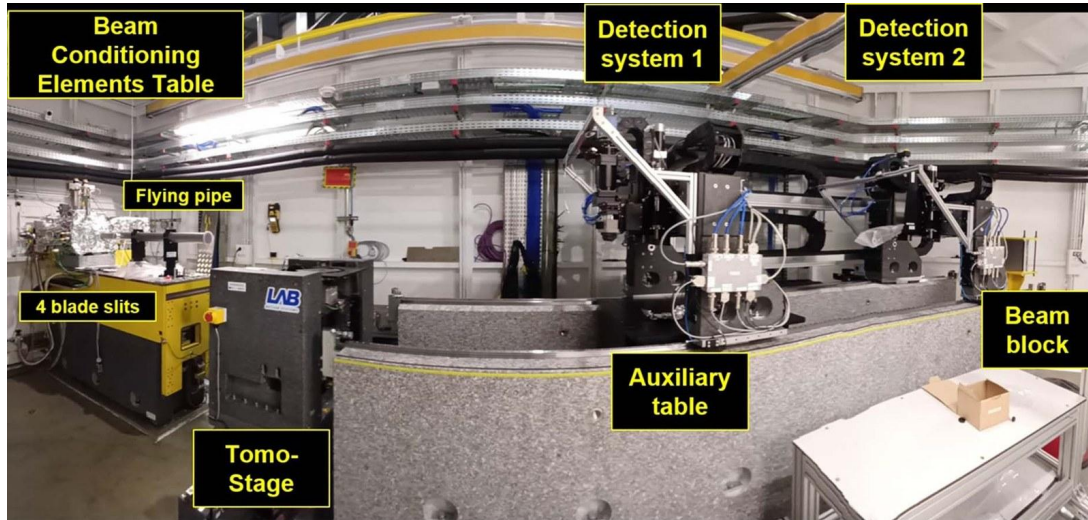
BL22 CLAEISS Experiment UI - what's next?

Connect GUI and MacroServer now both are running in the same python version:

- Allow to Start/Pause/Restart/Stop
- Show real progress
- Start from specific measure

Reuse it on BL16 Notos similar experiment measures.

BL31 Faxtor

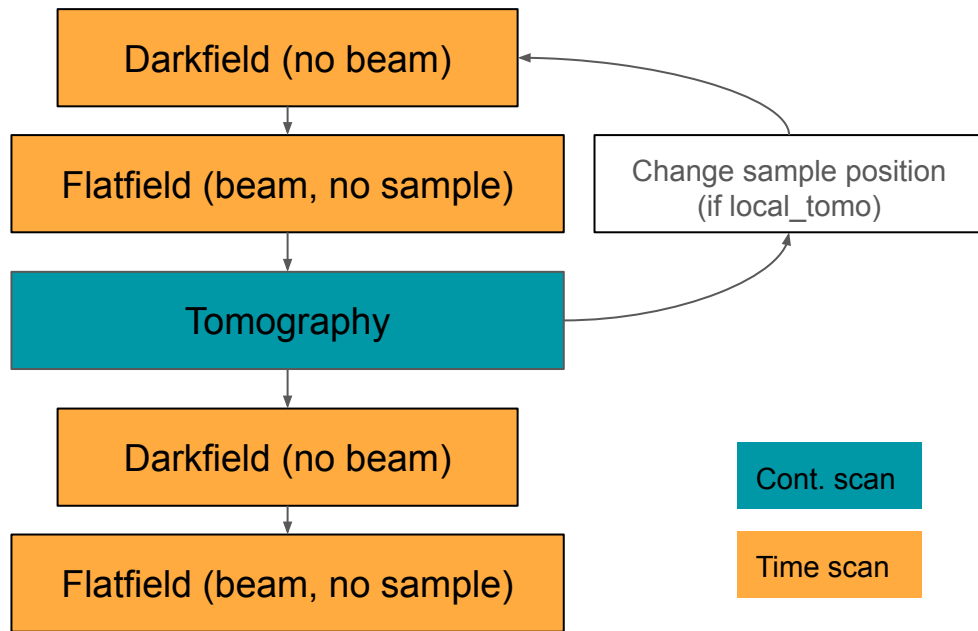


Camera	FPS
PCO.edge 4.2	100
PCO DiMaX CS4	1102
C-Blue	85
Phantom S710	5700

GONIO: ACS

BL31 Faxtor *Tomo Scan*

Sequence of scans:



Requirements:

- Handle fast shutter
- Asynchronous motor movements between scans
- Custom file storage
- Restart sequence from a given point
- Custom gonio behaviour:
 - Custom acceleration
 - Uninterrupted rotation

BL31 Faxtor *Tomo Scan*

- Scan configuration is serializable a Pydantic model

```
class TomoModel(BaseModel):
    tomo_steps: list[Step]
    current_slice_id: int =

class Step(BaseModel):
    sample_position: SamplePosition = SamplePosition()
    projections: int = Field(..., description="Number of images to take")
    exposure_time: Union[float, int] = Field(..., description="Time of the exposure")
    latency_time: Union[float, int] = Field(..., description="Time of the exposure")
    mode: Mode
    state: ScanState
    hooks: Dict = Field(default_factory=dict, exclude=True)
    point_id: int
    channel_refs: Dict[str, str] = Field(
        default_factory=dict,
        description="Key-value pairs for 2d channels and respective computed ref pattern"
    )
    gonio_scan: bool = False
    gonio_rotation: float = 180
```

BL31 Faxtor *Tomo Scan*

- Scan configuration is serializable a Pydantic model
- Scan can be stored and loaded from environment

Store

```
tomo_model = self.tomo_model.dict()  
self.setEnv(bl31.ENV_KEYS.TOMO_MODEL, tomo_model)
```

Load

```
model = TomoModel(**self.getEnv(bl31.ENV_KEYS.TOMO_MODEL))
```

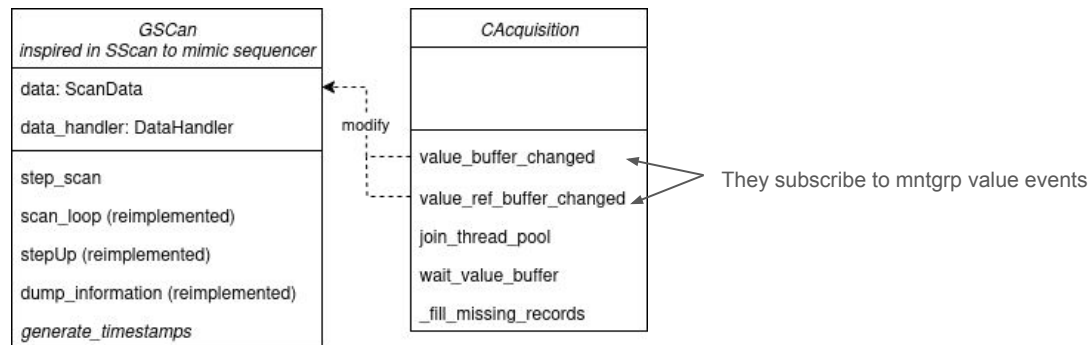
BL31 Faxtor *Tomo Scan*

- Scan configuration is serializable a Pydantic model
- Scan configuration can be stored and loaded from environment
- Scan configuration is updated at every step

```
def generator():  
    for step in tomo_model:  
        step.update(state=ScanState.Started)  
        save tomo_model to env  
        yield step  
        step.update(state=ScanState.Finished)  
        save tomo_model to env
```

BL31 Faxtor *Tomo Scan*

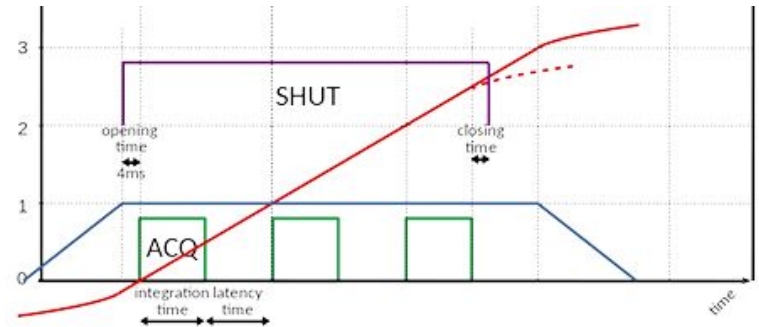
- Scan configuration is serializable a Pydantic model
- Scan configuration can be stored and loaded from environment
- Scan configuration is updated at every step
- Scan Framework API used:
 - Inherit from GScan and CAcquisition
 - We could reuse more code



Attributes and commands used or reimplemented from Scan API

BL31 Faxtor *Tomo Scan*: shutter

- Time to open and time to close is considered in order to avoid sample damage
- Uses **MultipleSynchDescription** and **Shutter** object
- Shutter in measurement group
- According to step, its TriggerGate Axis gets configured
 - Darkfield: disabled
 - Flatfield: master of camera
 - Tomo: slave of gonio, master of camera



BL31 Faxtor Tomography UI

File View Taurus Tools Help

Cycle:

Project_number:

Sample_index:

Experiment_index:

Measurement_index:

Detectors: ☒ pco_edge_image ☐ phantom_image ☐ twod01 ☐ sim_image

Set Next Sample Next Experiment

Mode: ☒ RAW ☐ ALIGNMENT

Tomo Local Tomo Timescan

Flatfield position (mm):

Number of projections:

Number of darkfields:

Number of flatfields:

Exposure time projections (s):

Darkfield exposure time (s):

Flatfield exposure time (s):

Jog axis: ☐

Repeat DF/FF: ☒

Latency (s):

gonio_rotation:

Run/Stop: tomo 0% Result: ☒ Progress StopMacro

1000 800 600 400 200 0 0 200 400 600 800 1000

Config Marker Data X Marker Data Y Marker Data I 1.000 s

MicroScope Shutters Breaks

Current Objective: 1

Magnification: 10x

Scintillator

Name: LuAg:Ce

Thickness: 0.0300

Units: um

DPad Controller

←: eh_tomo_mini_x
↑: eh_tomo_mini_y
t: gonio

0.30 0.10 0.00 0 3046.00

Microscope Table UP Tomo Stage OH Slits EH Slits

objective_selector	+	1.00	1.00 Abs
eh_microscope1_rt	+	0.25	-0.25 Abs
eh_microscope1_focus_1	+	-22.43	-22.43 Abs
eh_microscope1_focus_2	+	-24.23	-24.23 Abs
eh_microscope1_focus_3	+	-22.85	-22.85 Abs