

A Light for Science



mxCuBE Data Collection

European Synchrotron Radiation Facility

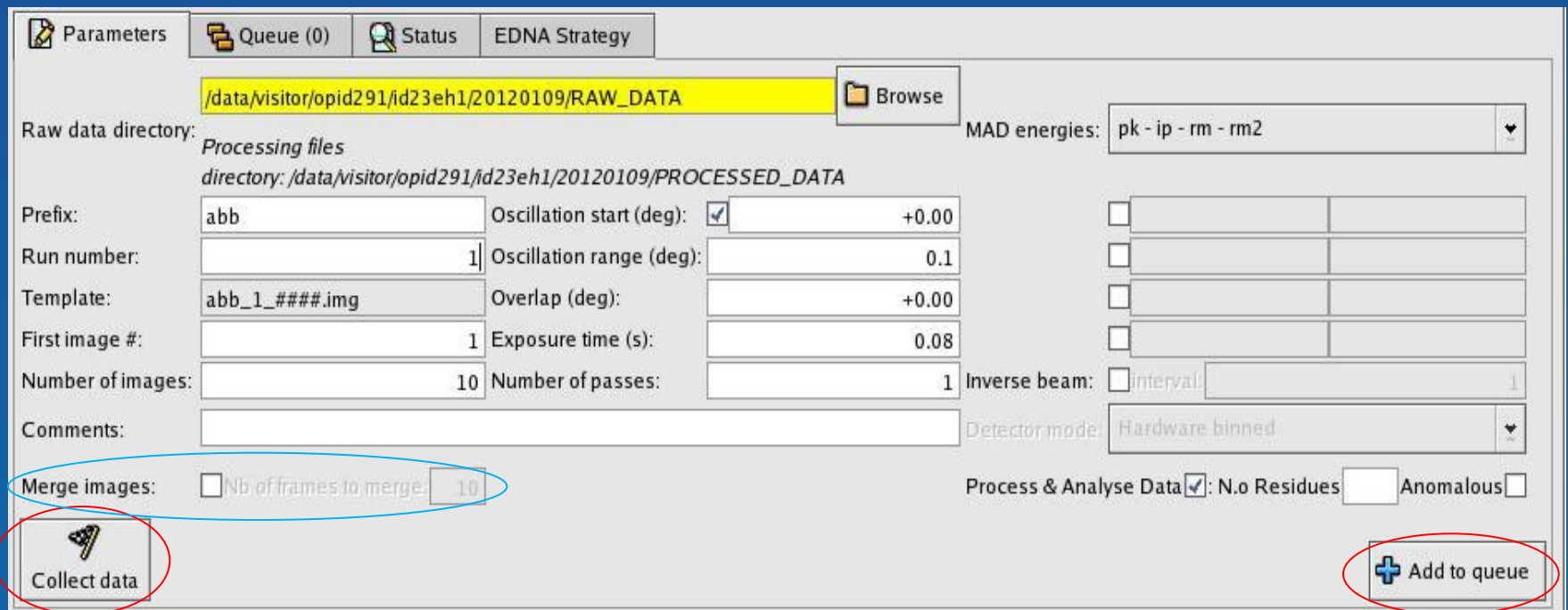
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Data Collection Sequence Handling

- Parameters settings - default and user defined
- Collection – single and multiple (queue) sequence
- EDNA Characterisation
- Shutterless data collection
- Special cases – helical data collection, 4D scan

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Parameters settings – DataCollectionParametersBrick



The screenshot shows the 'Parameters' tab of the DataCollectionParametersBrick interface. The 'Raw data directory' is set to `/data/visitor/opid291/fid23eh1/20120109/RAW_DATA`. The 'Processing files directory' is `/data/visitor/opid291/fid23eh1/20120109/PROCESSED_DATA`. The 'Prefix' is 'abb', 'Run number' is '1', 'Template' is 'abb_1_####.img', 'First image #' is '1', 'Number of images' is '10', 'Oscillation start (deg)' is '+0.00', 'Oscillation range (deg)' is '0.1', 'Overlap (deg)' is '+0.00', 'Exposure time (s)' is '0.08', 'Number of passes' is '1', 'MAD energies' is 'pk - ip - rm - rm2', 'Detector mode' is 'Hardware binned', 'Process & Analyse Data' is checked, 'N.o Residues' is checked, and 'Anomalous' is unchecked. The 'Merge images' checkbox is checked, and the 'Nb of frames to merge' is '10'. The 'Collect data' button is circled in red, and the 'Add to queue' button is also circled in red.

Parameters

Queue (0) Status EDNA Strategy

Raw data directory: `/data/visitor/opid291/fid23eh1/20120109/RAW_DATA` Browse

Processing files directory: `/data/visitor/opid291/fid23eh1/20120109/PROCESSED_DATA`

Prefix: `abb` Oscillation start (deg): ☒ +0.00

Run number: `1` Oscillation range (deg): `0.1`

Template: `abb_1_####.img` Overlap (deg): `+0.00`

First image #: `1` Exposure time (s): `0.08`

Number of images: `10` Number of passes: `1` Inverse beam: ☐ interval: `1`

Comments:

Detector mode: `Hardware binned`

Merge images: ☒ Nb of frames to merge: `10`

Process & Analyse Data ☒: N.o Residues ☒ Anomalous ☐

Collect data

+ Add to queue

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Data Collection – DataCollectQueueBrick

Parameters
Queue (3)
Status
EDNA Strategy

Run	Prefix	Start	Range	#images	Overlap	Time	Passes	Trans	Re
1	abb	+0.00	0.1	10	+0.00	0.08	1	100	
2	abb	+0.00	0.1	10	+0.00	0.08	1	100	
3	abb	+0.00	0.1	10	+0.00	0.08	1	100	

Load queue
Save queue
Collect queue

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Data Collection – DataCollectBrick2


Collect data

Confirm

Doing 1 oscillation over 1 sample, totaling 10 images.

Estimated time is 1 minute.

Warnings



The hutch hasn't been searched!

The centring isn't valid!

Options

☒ Generate processing input files
☐ Mount the sample using the sample changer
☐ Use helical oscillation
☐ Use scan4d oscillation
☐ Skip images already collected
☐ Take 4 snapshots of the sample before collecting

Files

Phi start	Phi end	Filename	Directory
0.0	0.1	abb_1_0001.img	/data/visitor/opid291/id23eh1/20120109/RAW_DATA
0.1	0.2	abb_1_0002.img	/data/visitor/opid291/id23eh1/20120109/RAW_DATA
0.2	0.3	abb_1_0003.img	/data/visitor/opid291/id23eh1/20120109/RAW_DATA

Continue

Cancel

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Data Collection – EDNARDBrick

Parameters
Queue (0)
Status
EDNA Strategy

Characterise using: 2 Images
☒ Account for Radiation Damage: of average protein Crystal

Data Collection Parameters

Run N.o: 1
Prefix: abb
Range: 0.1
Exposure: 0.08
Flux: ☐ ph/s 3e+12

Sample

Maximum vertical crystal dimension, mm: 0.1
Minimum vertical crystal dimension, mm: 0.1
Radiation Susceptibility: 1.0

Collect and Characterise

Diffraction Plan

Optimized SAD: ☐
Induce Bum Strategy: ☐
Force Space Group: ☐ Group P1
Strategy Complexity: single subwedge
Maximum exposure time per data collection Time(secs): 6000.0
Aimed I over Sigma at highest Resolution: 3.0
Define Aimed Resolution (default - highest possible): ☐ Angstroms 3.0
Define Aimed Completeness (default >= 0.99): ☐ (0.0-0.99) 0.99
Define Aimed Multiplicity (default - optimized) : ☐ 4.0

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- Control – Datacollect hardware object

```
<procedure class="DataCollect">
  <specversion>lid292:exp</specversion>
  <command type="spec" name="macroCollect">datacollection</command>
  <command type="spec" name="collectCleanup">datacollection_cleanup</command>
  <command type="spec"
    name="macroValidateParameters">validate_collect_parameters</command>
  <channel type="spec" name="arguments">datacollection_parameters</channel>
  <channel type="spec" name="imageCollected">CURRENT_IMAGE</channel>
  <channel type="spec" name="stopscan">STOP_COLLECT_LOOP</channel>
  <channel type="spec" name="messages">eprodc_log_message</channel>
  <channel type="spec" name="fatalCollect">eprodc_fatal_collect</channel>
  <channel type="spec" name="xdsFile">XDS_INPUT_FILENAME</channel>
```

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```
<directoryprefix>id29</directoryprefix>  
<mxlocal>/mxlocal</mxlocal>  
<safetyshutter>/safshut</safetyshutter>  
<resmotor>/exp/res</resmotor>  
<samplechanger>/sc</samplechanger>  
<minidiff>/udiff</minidiff>  
<slitbox>/slitbox</slitbox>  
<machcurrent>/mach</machcurrent>  
<cryostream>/cryospy</cryostream>  
<energyscan>/energyscan</energyscan>  
<detdistmotor>/exp/DtoX</detdistmotor>  
<transmission>/attenuators</transmission>  
<autoProcessingServer>localhost:23640</autoProcessingServer>  
</procedure>
```


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- Control – non spec equipment

```
<device class = "Shutter">  
  <username>SafShut</username>  
  <taconame>id29/bsh/1</taconame>  
  <interval>2000</interval>  
</device>
```

- Control – spec equipment

```
<device class = "SpecMotor">  
  <username>Resolution</username>  
  <specname>res</specname>  
  <specversion>lid292:exp</specversion>  
</device>
```

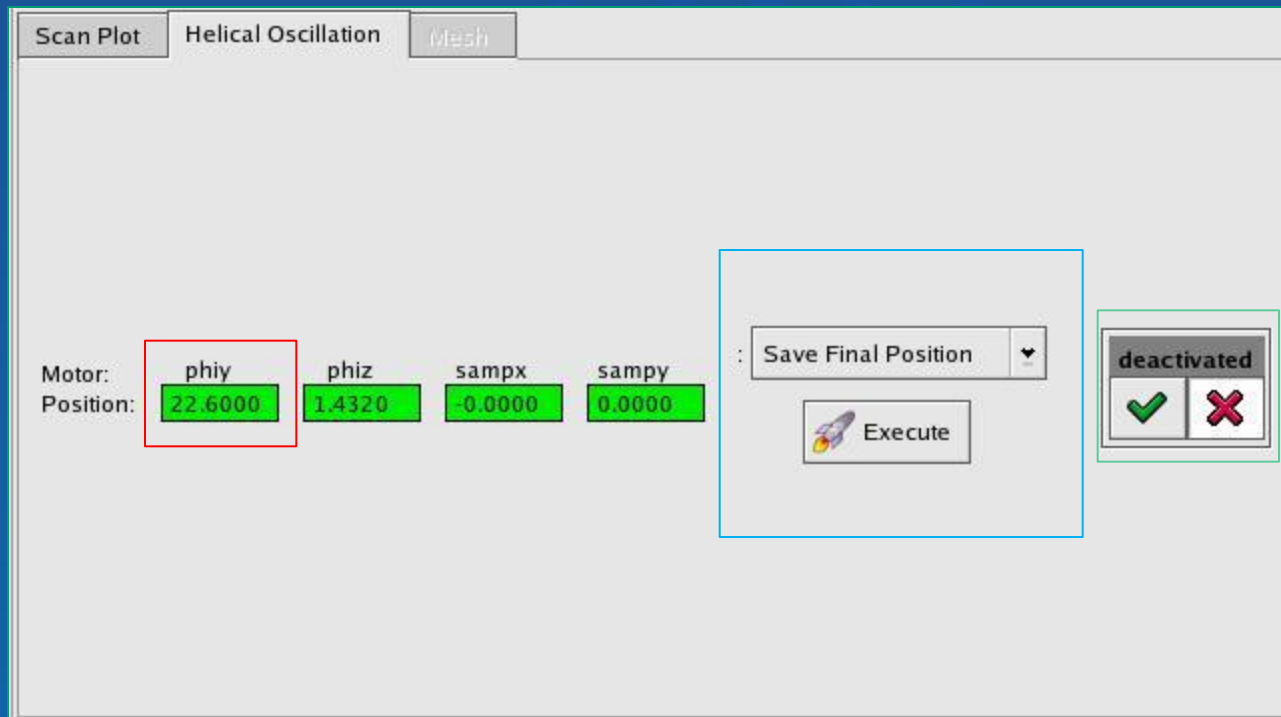
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mxlocal.xml – example of local parameters used to change the DataCollectionParametersBrick appearance

```
<beamline_pars>
...
  <BCM_PARS>
    ...
    <detector>
      <type>pilatus</type>
      <model>6M</model>
      <px>0.172</px>
      <py>0.172</py>
    </detector>
  </BCM_PARS>
</beamline_pars>
```

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Helical data collection



Label, Spacer, **SpecValueBrick**, **CommandBrick**, **DuoStateBrick**

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Helical data collection

```
<device class="InOut">
  <username></username>
  <specversion>lid292:exp</specversion>
  <command type="spec" name="set_out">helical_oscil_off</command>
  <command type="spec" name="set_in">helical_oscil_on</command>
  <channel type="spec" name="state">HELICAL_OSCIL</channel>
  <offset>0</offset>
</device>

<procedure class="MultiCollect">
  <datacollect>/datacollect</datacollect>
  <channel type="spec" version="lid292:exp" name="helical">HELICAL_OSCIL</channel>
  <channel type="spec" version="lid292:exp" name="detector">MXBCM_PARS["detector"]["type"]</channel>
  <channel type="spec" version="lid292:exp" name="shutterless">PILATUS_SHUT</channel>
  <channel type="spec" version="lid292:exp" name="scan4d">HELICAL_SCAN4D</channel>
</procedure>
```

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Helical data collection

```

<procedure>
  <specversion>lid292:exp</specversion>
  <command> <type>spec</type><name>Execute</name>
    <argument><name></name><type>combo
      <item><name>Save Final Position</name><value>2</value></item>
      <item><name>Save Start Position</name><value>1</value></item>
      <item><name>Go To Final Position</name><value>22</value></item>
      <item><name>Go To Start Position</name><value>11</value></item>
      <item><name>Reset All Positions</name><value>99</value></item>
    </type></argument>
  <toexecute>helical_getpos</toexecute>
</command>
</procedure>

```

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4Dscan data collection

- Only available with MD2 hardware/device server
- Used with shutterless pilatus to replace the helical data collection.

```
<device class="InOut">
  <username></username>
  <specversion>lid292:exp</specversion>
  <command type="spec" name="set_out">helical_scan4d_off</command>
  <command type="spec" name="set_in">helical_scan4d_on</command>
  <channel type="spec" name="state">HELICAL_SCAN4D</channel>
  <offset>0</offset>
</device>
```

But :

- Could be used for mesh scan by using the queue to pass parameters to the collection procedure

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Conclusion



- Relatively easy to add missing parameters
- Reuse of a Brick only by changing the hardware object
- Signal mechanism allows good flexibility.



- Strongly tight to spec – hardware objects need refactoring
- Signal mechanism difficult to follow – only visible in the GUI builder