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Ezequiel Panepucci :: Software Engineer :: Paul Scherrer Institut

DA+ Complex Protocols Made Easy for Macromolecular Crystallography at the Swiss Light Source

ICALEPS 2015, Melbourne, VIC, Australia

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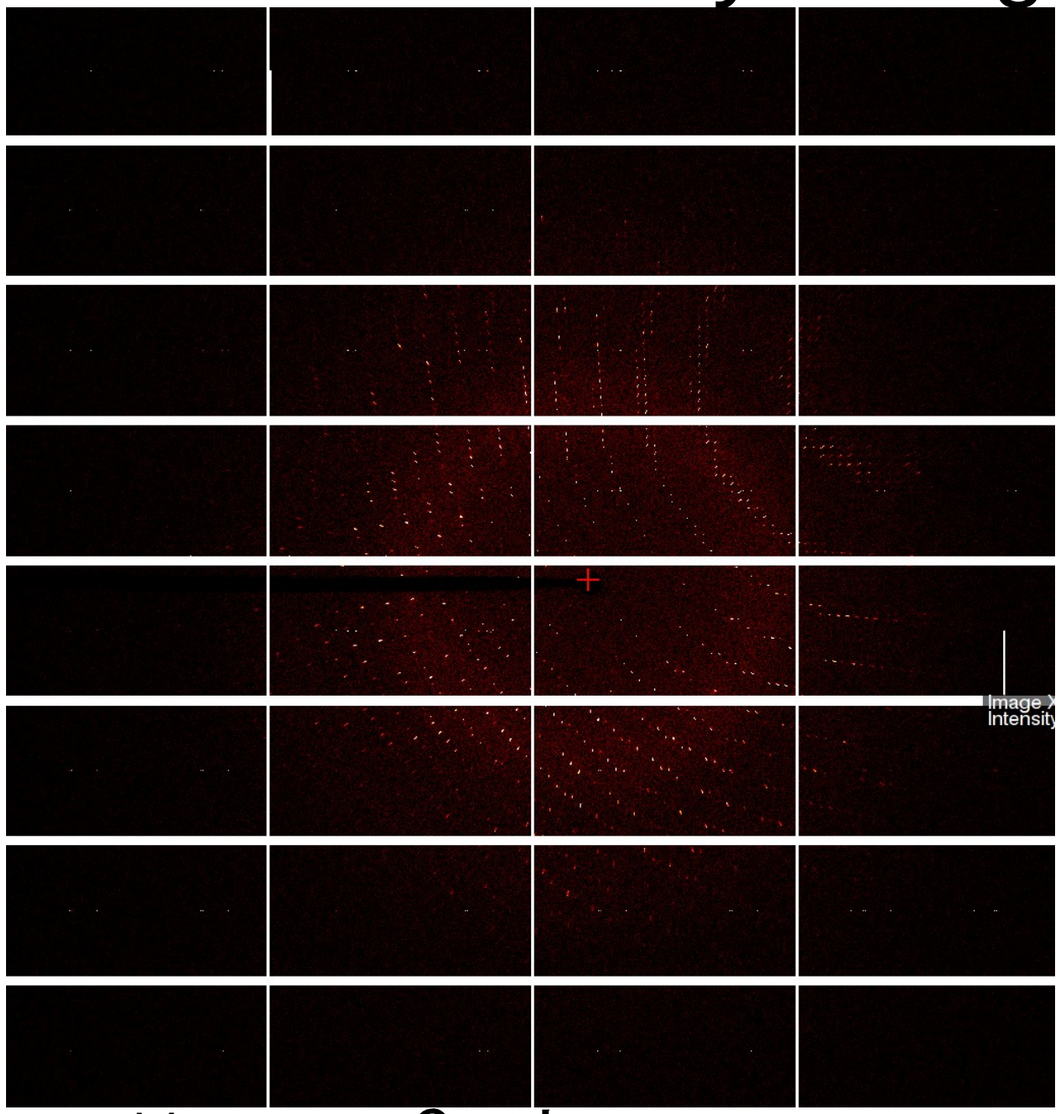
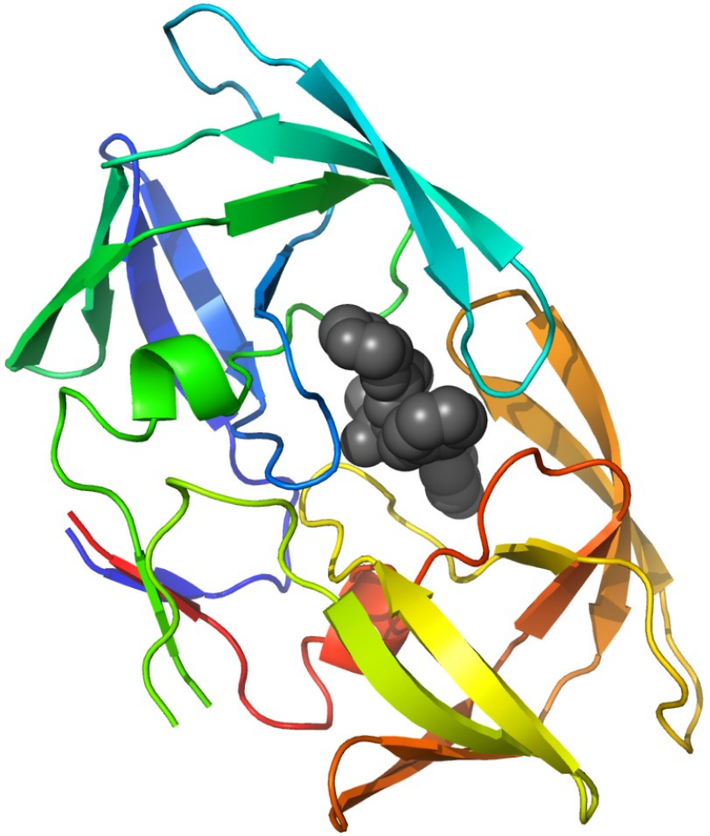
Macromolecular Crystallography

100s to 1000s of these



Many of these



This one

SLS MX Beamlines

	Focused Spot Size (um)	Flux at 12.4 keV 400 mA (ph/s)	Energy Range (KeV)	Source	Detector (Gonio)
X06SA	5x5 – 80x80 Focus on det.	> $2x10^{12}$	5.7 – 17.5	U19	EigerX 16M (single axis)
X10SA	50x10 10x10 apert.	> $2x10^{12}$	6 – 20	U19	Pilatus 6MF (single axis)
X06DA	80x45	~ $5x10^{11}$	6 – 17.5	Superbend magnet	Pilatus 2MF (multi-axis: prigo)

All beamlines fitted with Irelec CATS.
All beamlines to be upgraded with a multi-axis SmarGon goniometer from SmarAct.

Some of the gadgets we need to cope with

I speak Aerobasic via EPICS

I speak with sockets

I do sockets as well!

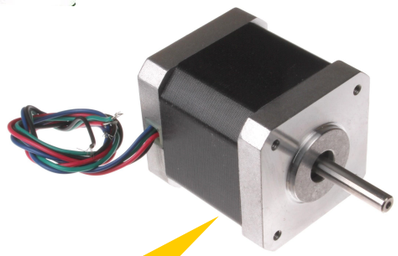
I speak EPICS

I speak EPICS

I speak EPICS

I speak EPICS

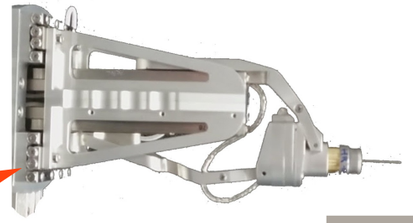
I speak EPICS



I speak EPICS

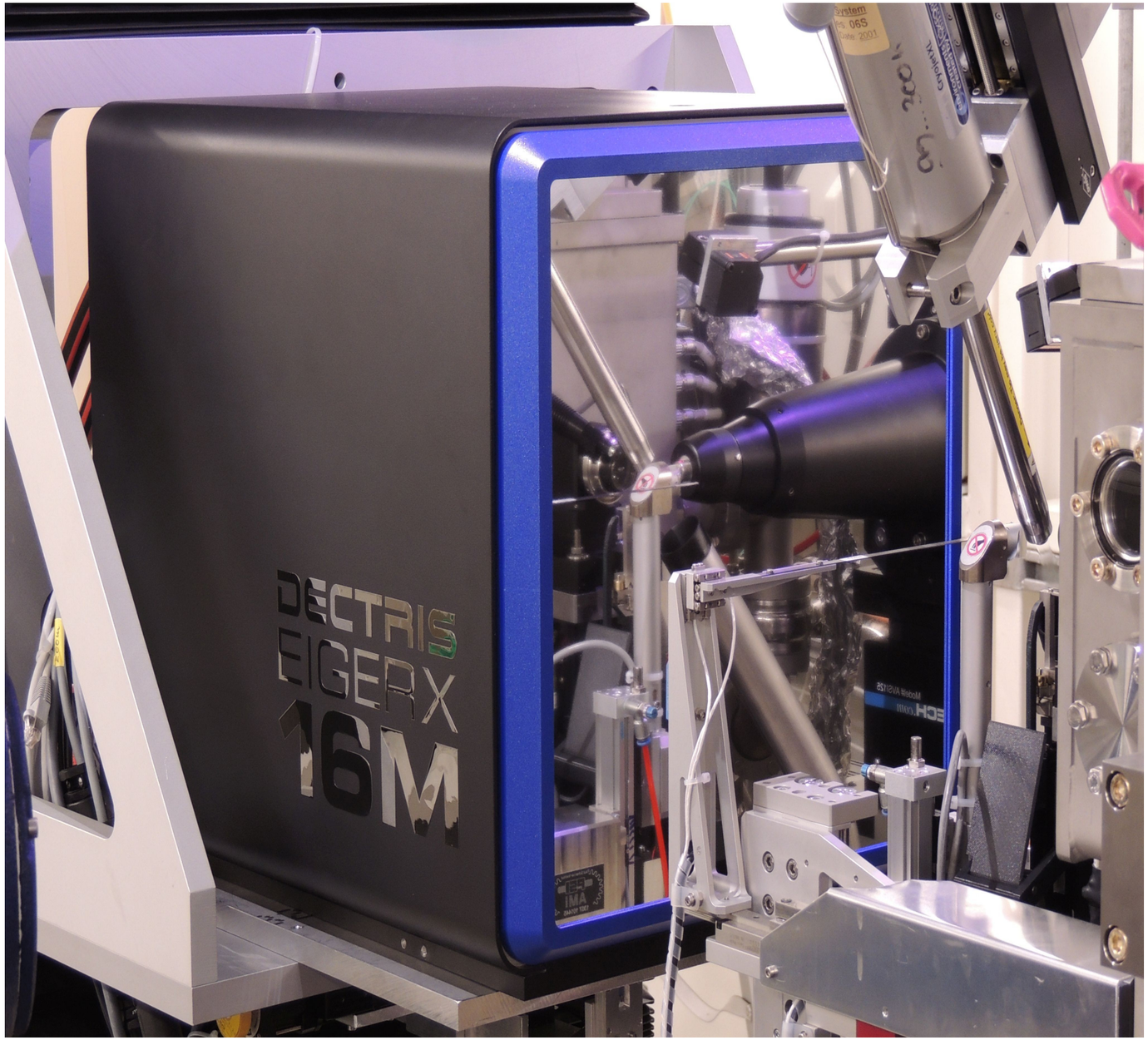
I speak EPICS

I speak Delta Tau Via telnet

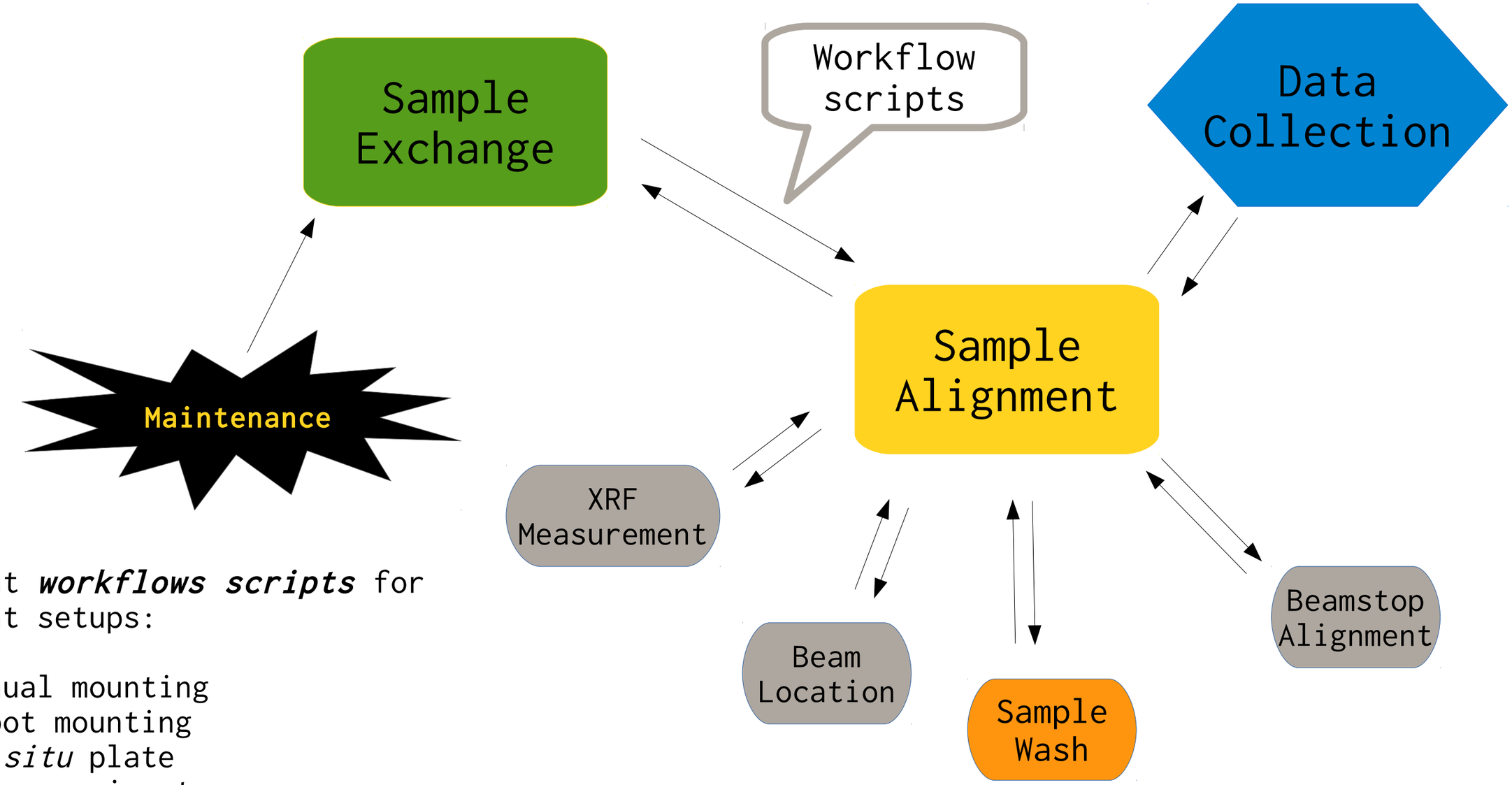


Non exhaustive, ever changing list.

Socializing gadgets



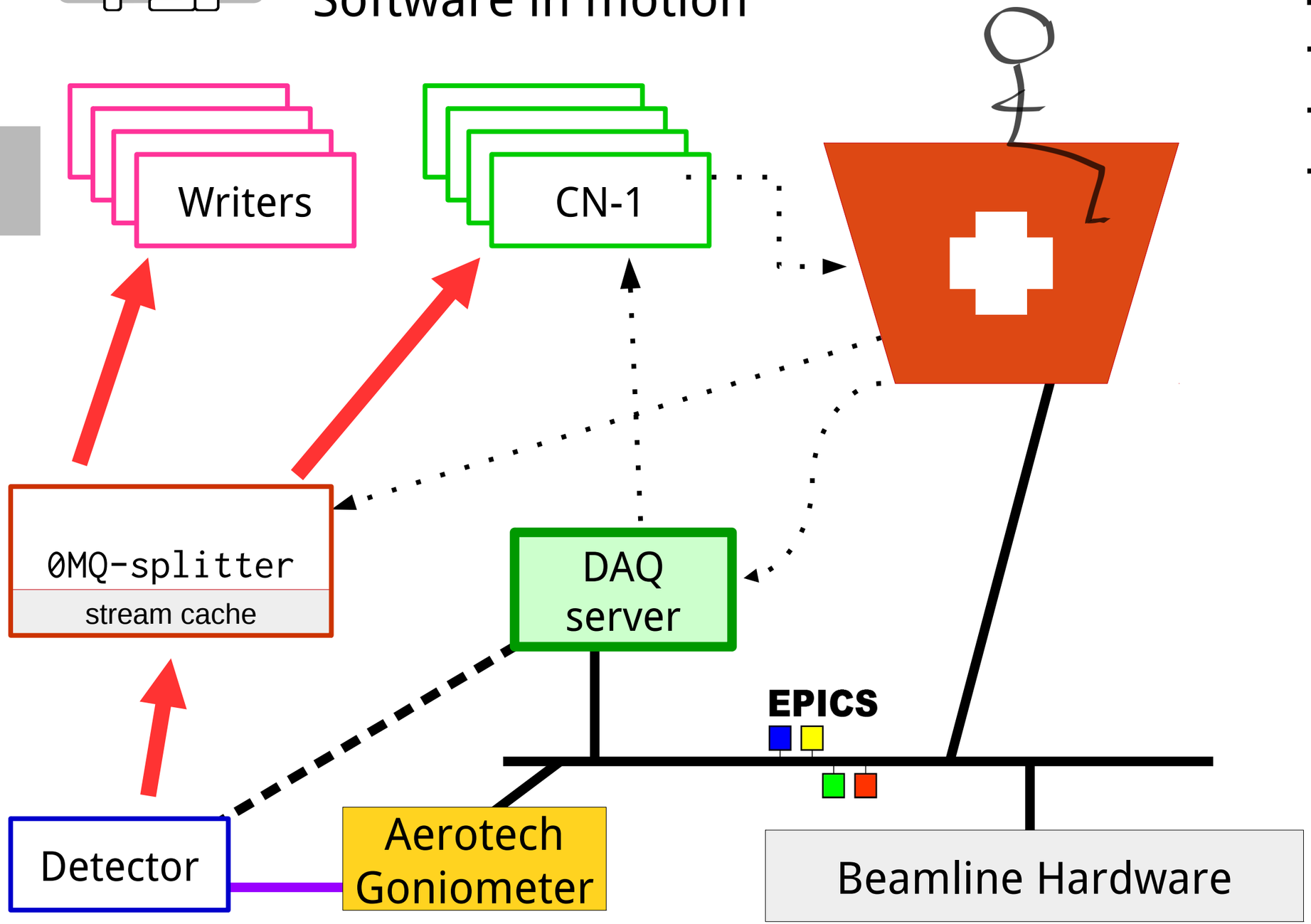
Escape: our beamline state machine



Different ***workflows scripts*** for different setups:

* Manual mounting
* Robot mounting
* *In situ* plate
* Jet experiments
* No Movements

Software in motion



Languages

- Java
- Python
- Aerobasic

Active MQ
0MQ
REST
TTL

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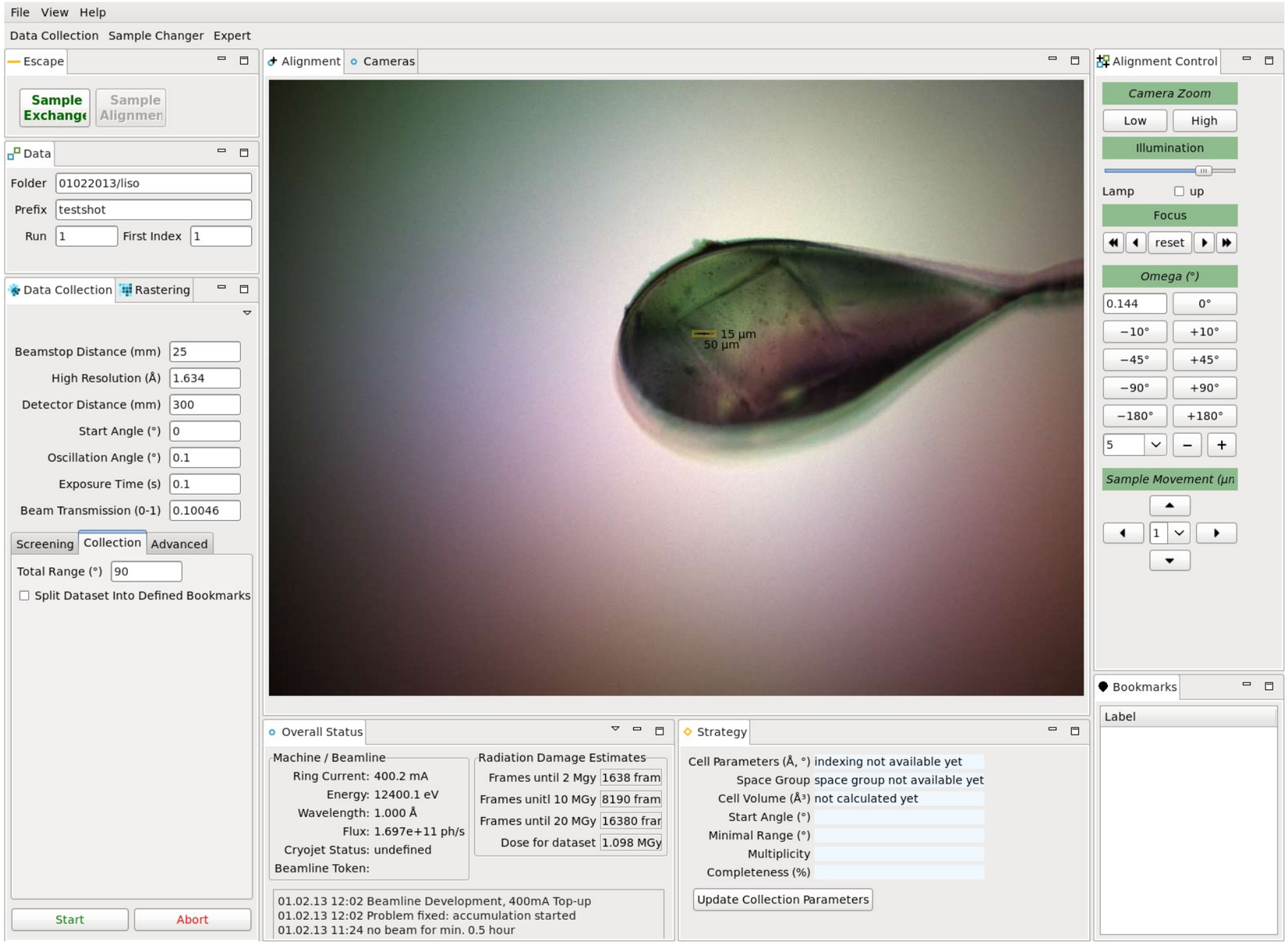
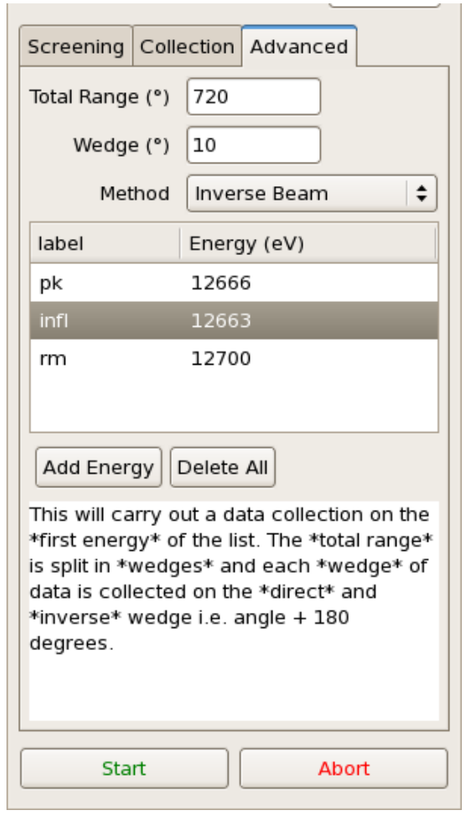
User Interface





Sequencer examples

Scan Request


```
{
'method': 'helical',
'beamTransmission': None,
'exposureTime': 0.1,
'firstIndex': 1,
'folder': u'zac/test',
'omega': 0.0,
'oscillationAngle': 0.1,
'points': [
          [-18.6, 0.1, 0.4],
          [-18.58, 0.1, 0.4]
         ],
'prefix': u'testshot',
'runNumber': 1,
'startAngle': 0.0,
'trackingId': u'test-track',
'totalRange': 90.0
 }
```


Individual Scans


```
[

{'first_index': 1,
  'folder': u'zac/test',
  'num_frames': 450,
  'prefix': u'testshot',
  'run': 1,
  'sample_xyz': (-18.6, 0.1, 0.4),
  'start_angle': 0.0},

 {'first_index': 451,
  'folder': u'zac/test',
  'num_frames': 450,
  'prefix': u'testshot',
  'run': 1,
  'sample_xyz': (-18.58, 0.1, 0.4),
  'start_angle': 45.0}

]
```

Multiple Anomalous Diffraction Request

Scan Request

```
{
'method': 'interleave_and_inverse_first',
'exposureTime': 0.1,
'firstIndex': 1,
'folder': u'test',
'omega': 0.0,
'oscillationAngle': 0.1,
'energies': [
     ['peak', 8888.0],
     ['infl', 11111.0]
          ],
'prefix': u'testshot',
'runNumber': 1,
'startAngle': 0.0,
'trackingId': u'test-track',
'totalRange': 90.0,
'wedge': 45.0,
 }
```

Individual Scans

```
{'energy': 8888.0,
  'first_index': 1,
  'folder': u'test/8888eV',
  'num_frames': 450,
  'prefix': u'testshot_8888eV',
  'run': 1,
  'start_angle': 0.0},

 {'energy': 8888.0,
  'first_index': 1,
  'folder': u'test/8888eV',
  'num_frames': 450,
  'prefix': u'testshot_8888eV_inv',
  'run': 1,
  'start_angle': 180.0},

 {'energy': 11111.0,
  'first_index': 1,
  'folder': u'test/11111eV',
  'num_frames': 450,
  'prefix': u'testshot_11111eV',
  'run': 1,
  'start_angle': 0.0},
```

```
{'energy': 11111.0,
 'first_index': 451,
 'folder': u'test/11111eV',
 'num_frames': 450,
 'prefix': u'testshot_11111eV',
 'run': 1,
 'start_angle': 45.0},

{'energy': 8888.0,
 'first_index': 451,
 'folder': u'test/8888eV',
 'num_frames': 450,
 'prefix': u'testshot_8888eV',
 'run': 1,
 'start_angle': 45.0},

{'energy': 8888.0,
 'first_index': 451,
 'folder': u'test/8888eV',
 'num_frames': 450,
 'prefix': u'testshot_8888eV_inv',
 'run': 1,
 'start_angle': 225.0}
```

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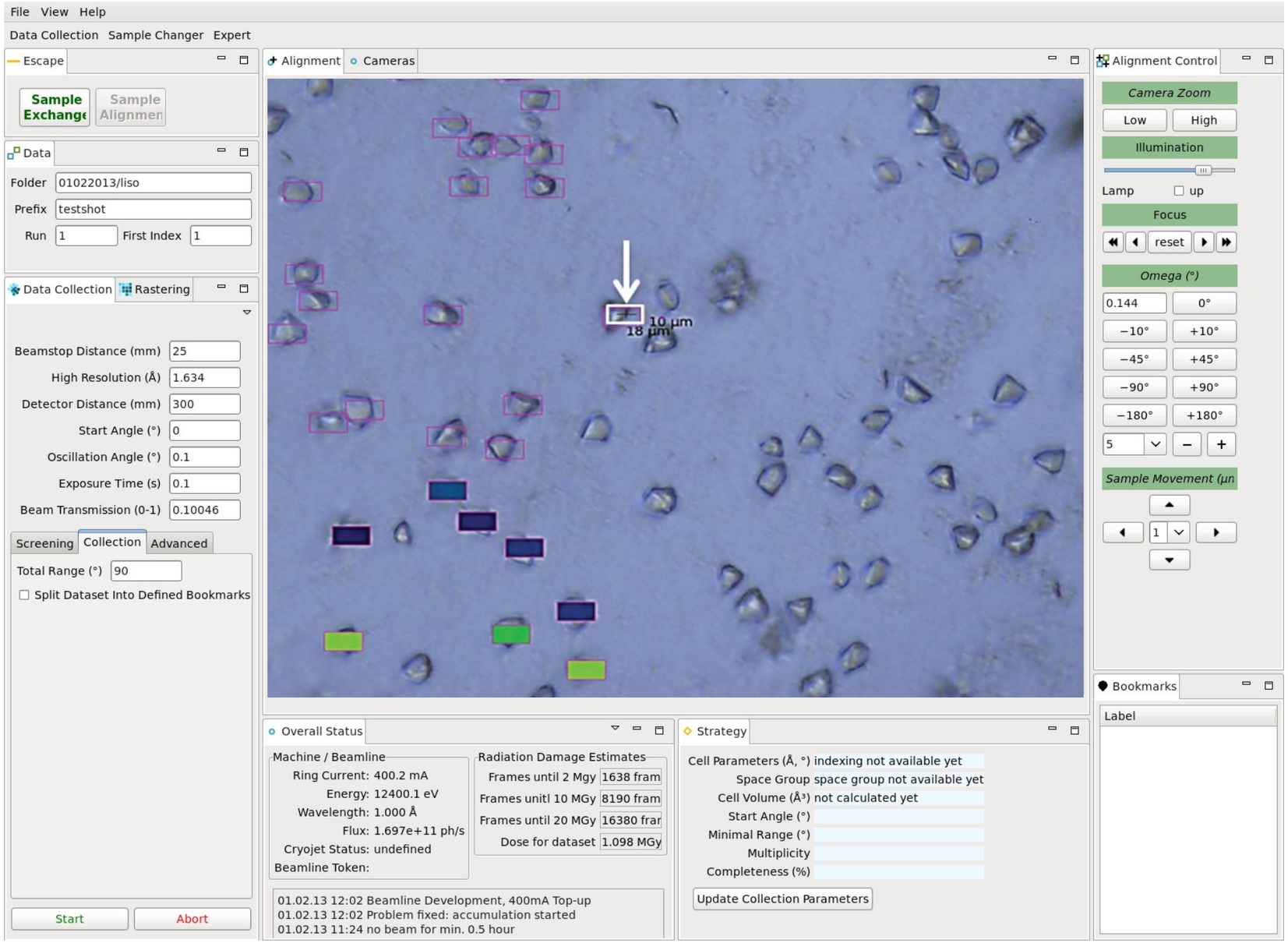
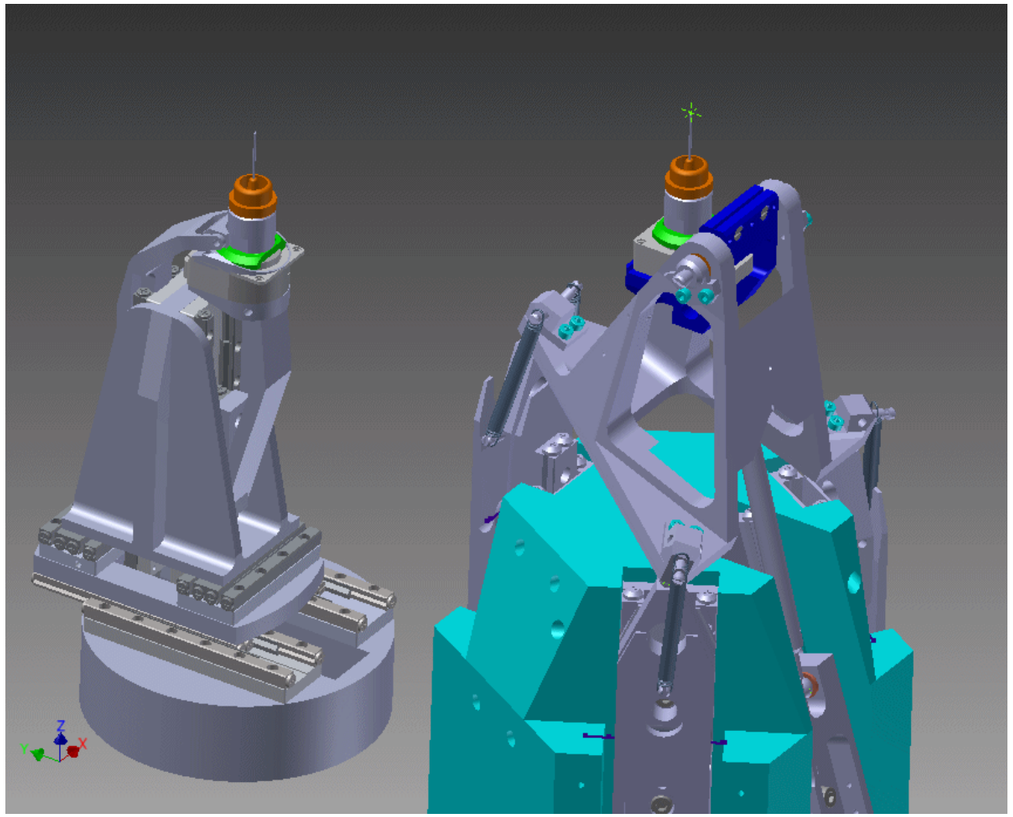
In situ minisets



Sample Movers: multi-axis

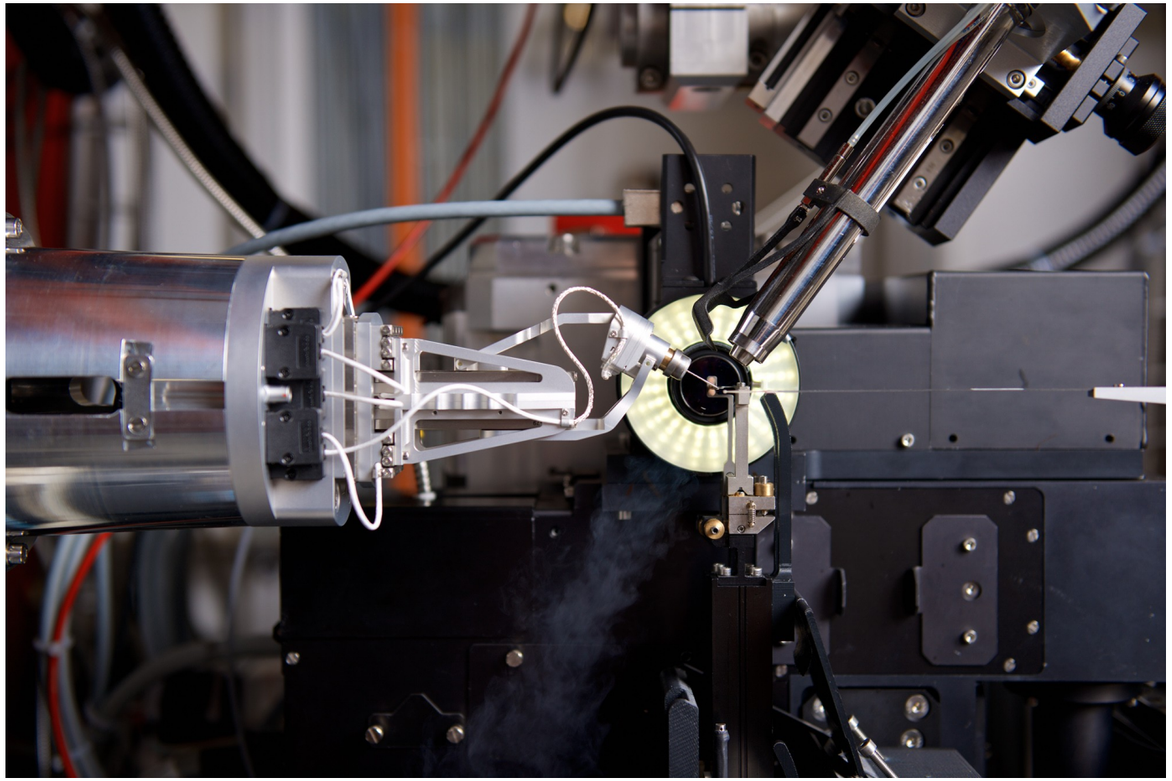
SmarGon PRIGo



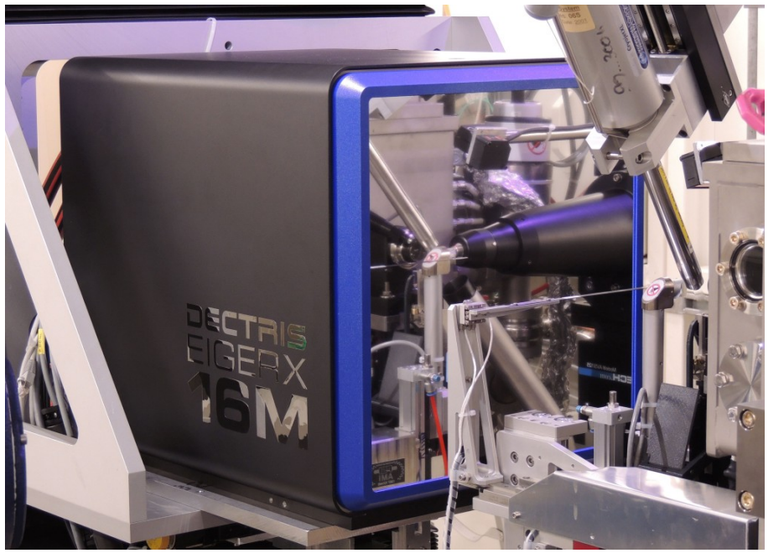
DeltaTau C.S. Orchestra C.S.

5 um SoC

SmarGon



Detectors



Dectris EigerX 16M

* REST API
* 133 Hz
* 75 um pixel size
* Data: ZMQ or HDF5

Pilatus 6MF & 2MF

* Socket API
* 25 Hz & 60Hz
* 172 um pixel size
* Data: CBF files

Summary

- Messaging decouples components very effectively
- The **escape** state machine centralizes coordinated motion improving safety
- Users appreciate a **keep-it-simple** approach

Acknowledgements

Controls

- Simon Ebner
- Jose Gabadinho
- Xiaoqiang Wang

IT

- Heiner Billich

MX Group

- Meitian Wang – group leader
- Justyna Wojdyla – scientist
- All my colleagues
- Our Users for testing...

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The End