



WIR SCHAFFEN WISSEN - HEUTE FÜR MORGEN

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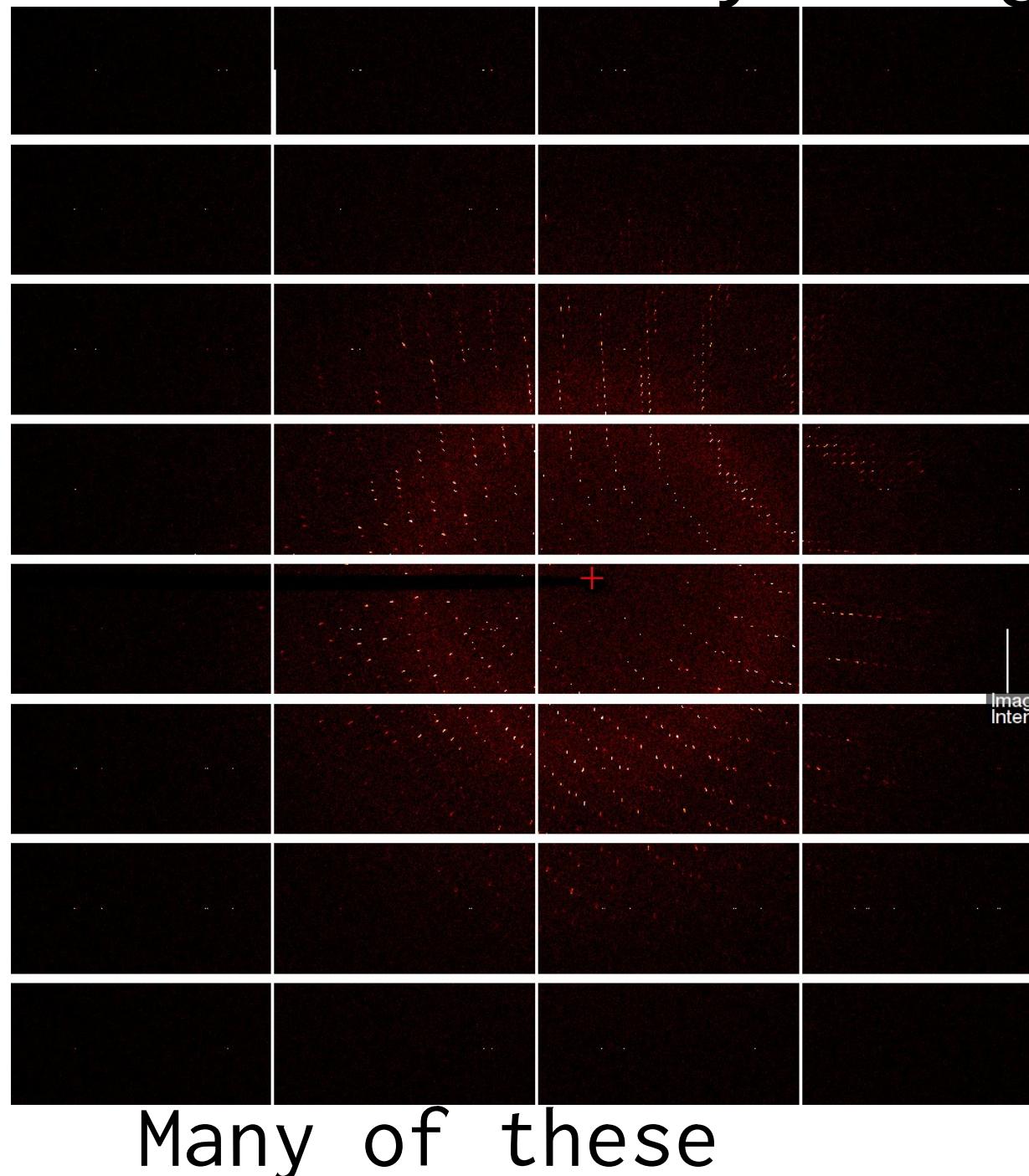
DA+ Complex Protocols Made Easy for Macromolecular Crystallography at the Swiss Light Source

ICALEPS 2015, Melbourne, VIC, Australia

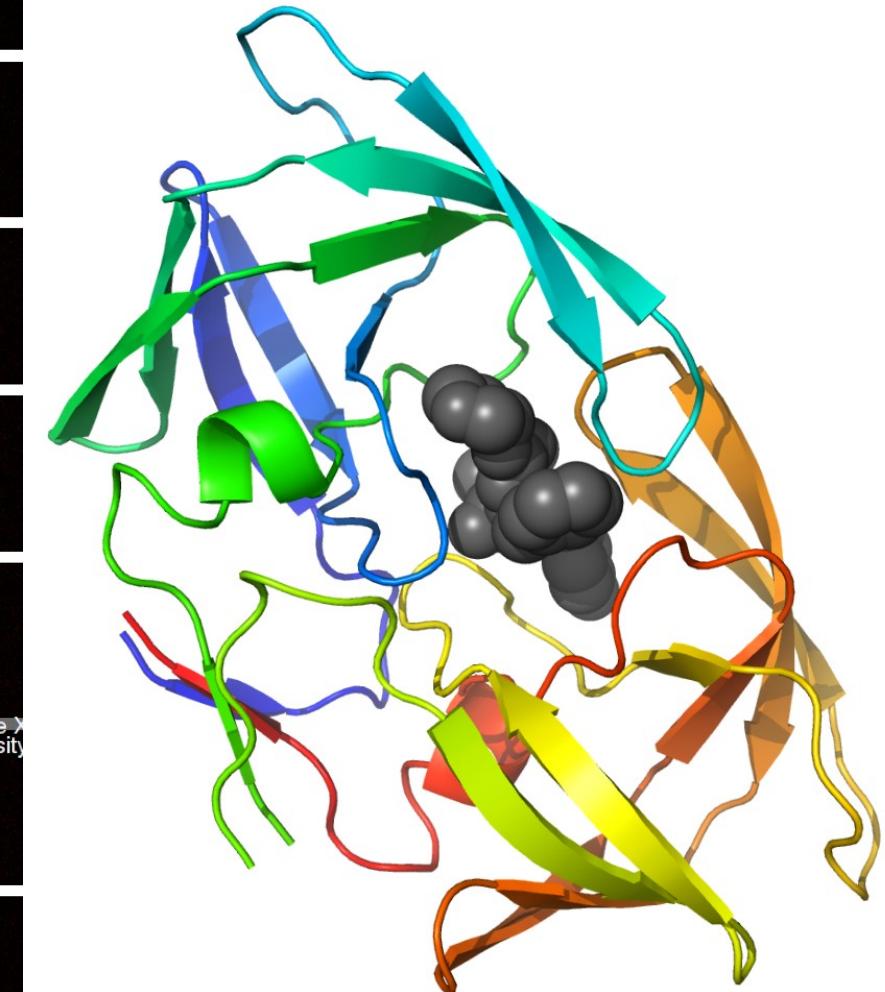
# Macromolecular Crystallography



100s to 1000s  
of these



Many of these



This one

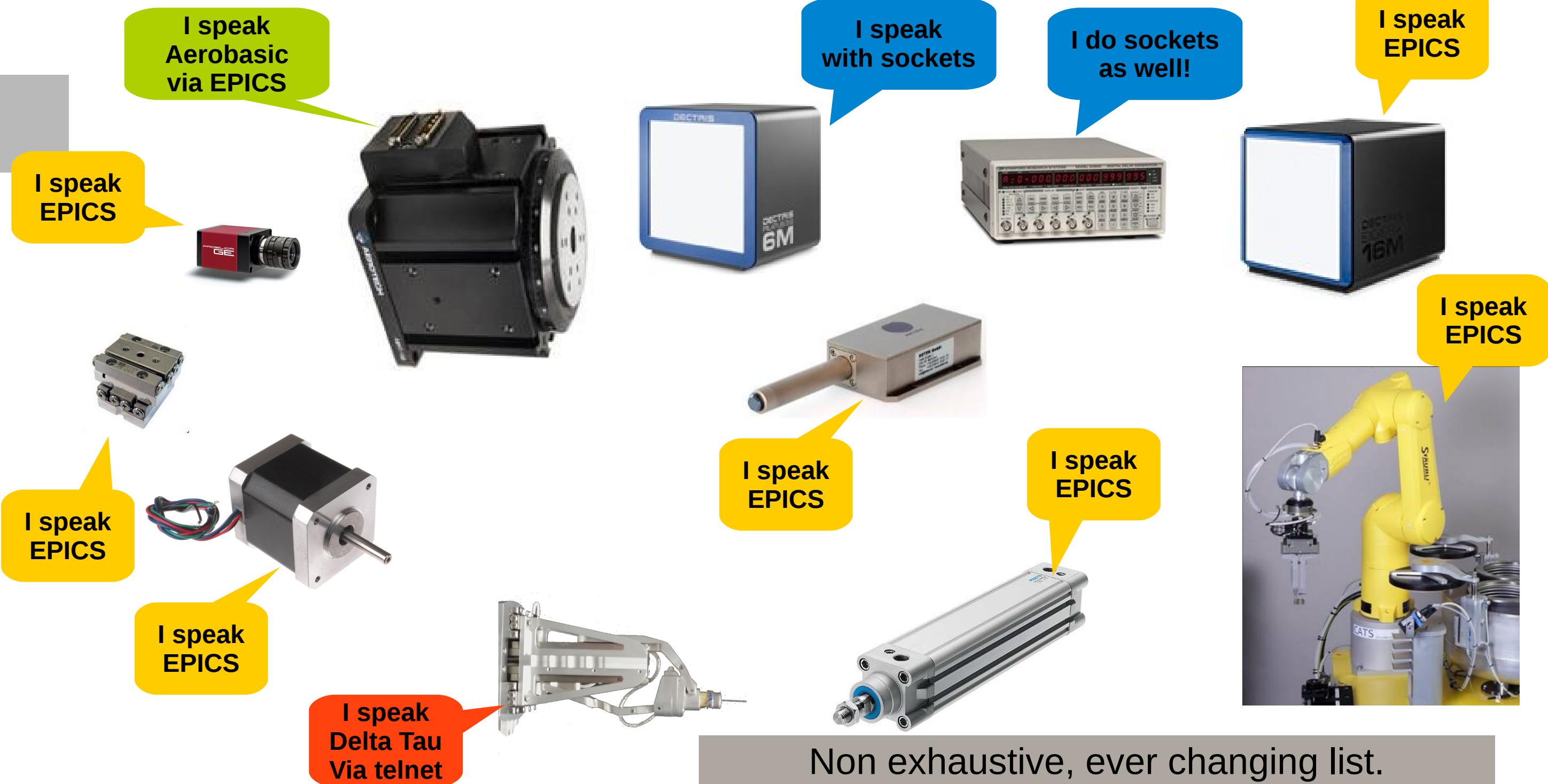
# SLS MX Beamlines

	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.	> $2 \times 10^{12}$	5.7 – 17.5	U19	EigerX 16M (single axis)
X10SA	50x10 10x10 apert.	> $2 \times 10^{12}$	6 – 20	U19	Pilatus 6MF (single axis)
X06DA	80x45	~ $5 \times 10^{11}$	6 – 17.5	Superbend magnet	Pilatus 2MF (multi-axis: prigo)

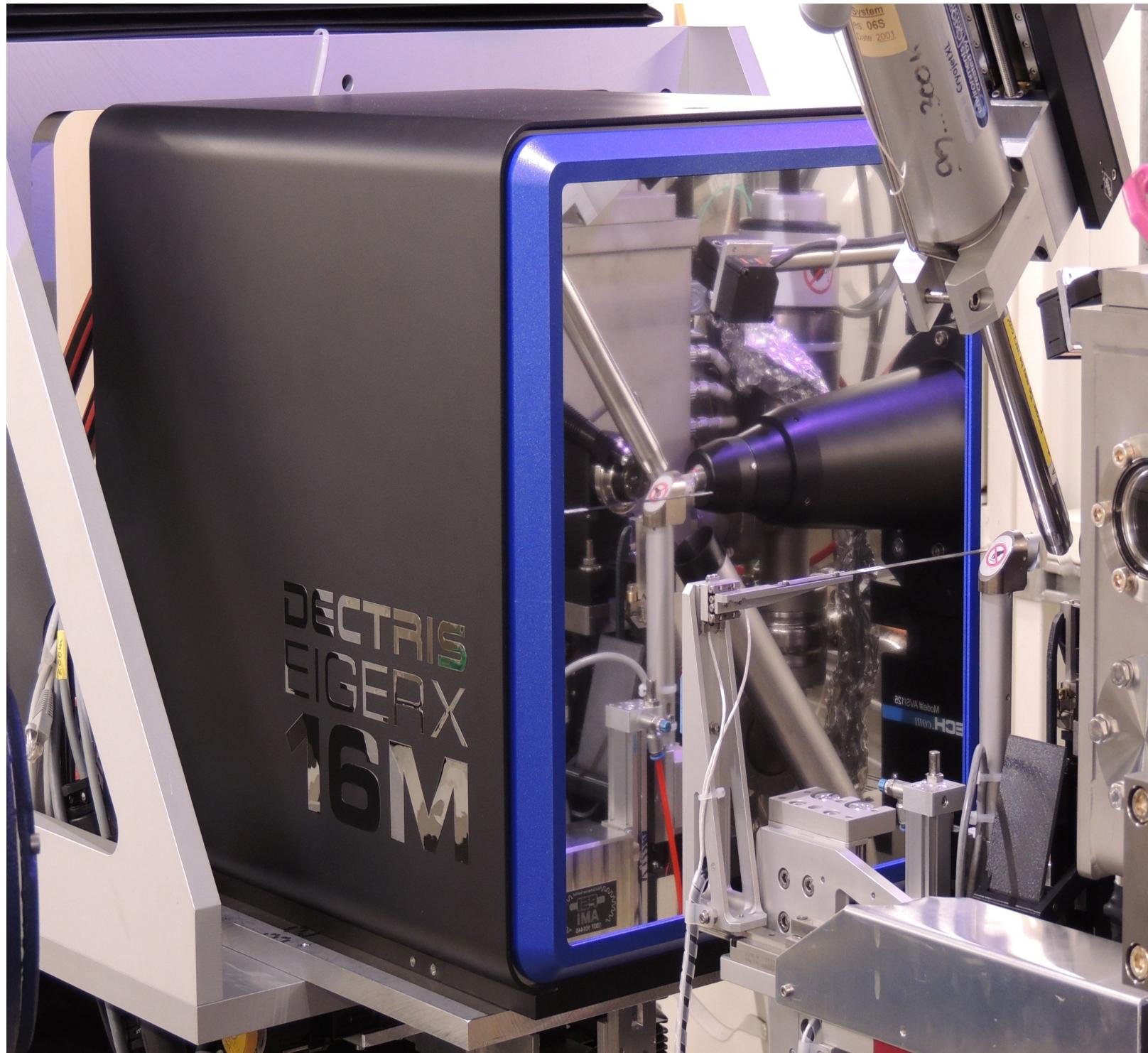
All beamlines fitted with Irelec CATS.

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

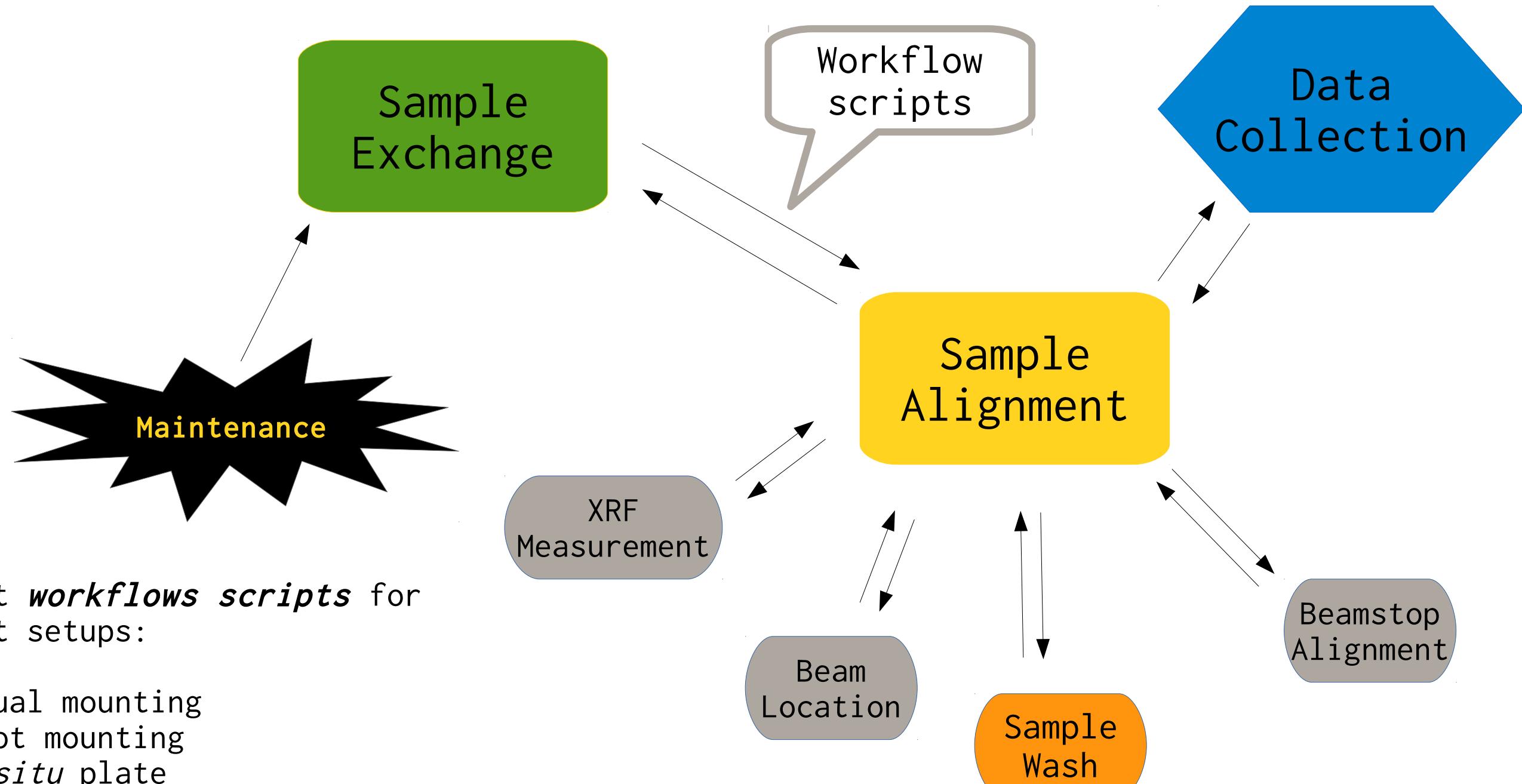
# Some of the gadgets we need to cope with



# Socializing gadgets



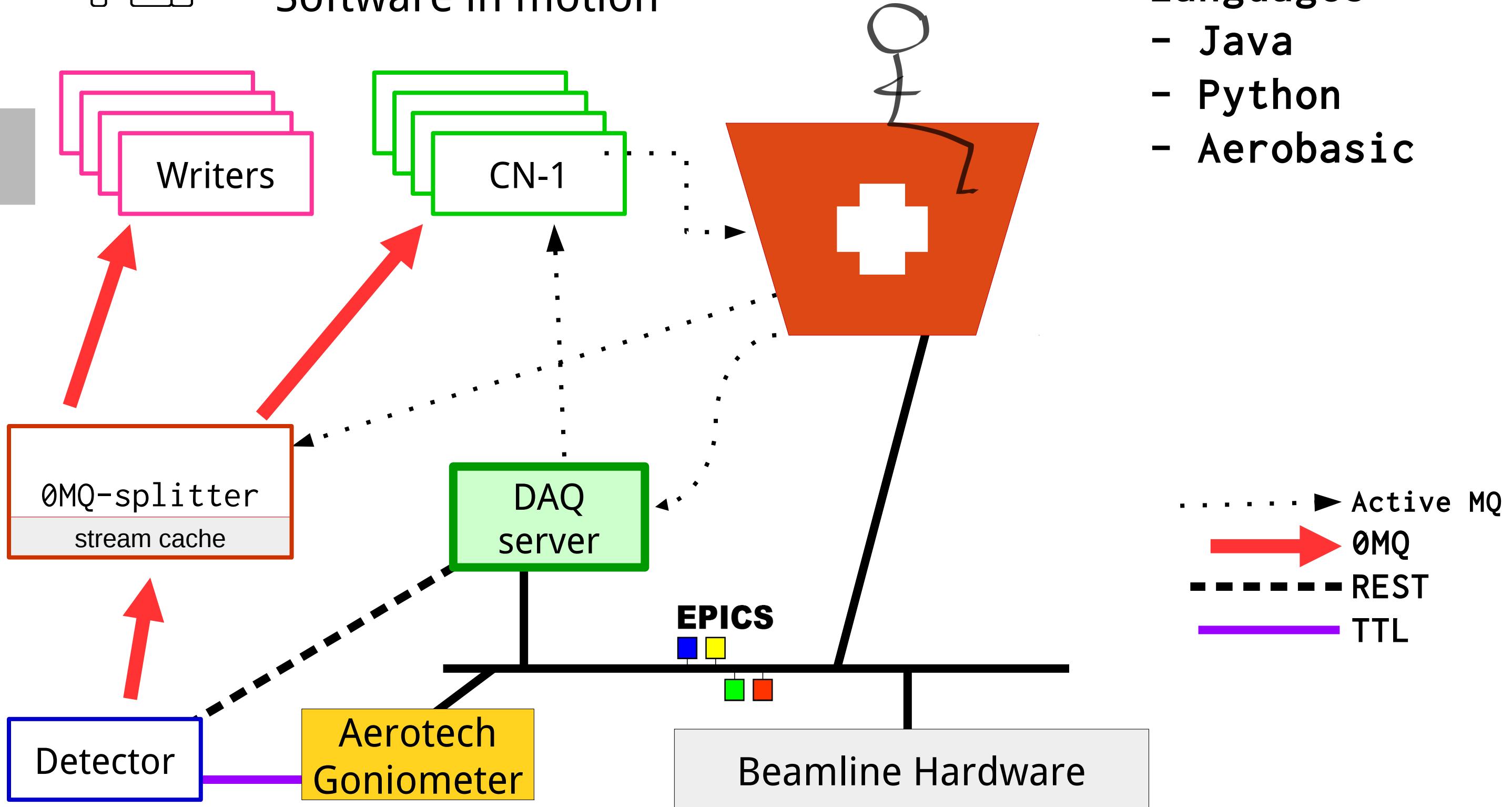
# Escape: our beamline state machine



Different **workflows scripts** for different setups:

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

# Software in motion



# User Interface

**File View Help**

**Data Collection Sample Changer Expert**

**Alignment** **Cameras**

**Sample Exchange** **Sample Alignment**

**Data**

Folder: 01022013/liso  
Prefix: testshot  
Run: 1 First Index: 1

**Data Collection Rastering**

Beamstop Distance (mm): 25  
High Resolution (Å): 1.634  
Detector Distance (mm): 300  
Start Angle (°): 0  
Oscillation Angle (°): 0.1  
Exposure Time (s): 0.1  
Beam Transmission (0-1): 0.10046

**Screening Collection Advanced**

Total Range (°): 90  
 Split Dataset Into Defined Bookmarks

**Overall Status**

Machine / Beamline  
Ring Current: 400.2 mA  
Energy: 12400.1 eV  
Wavelength: 1.000 Å  
Flux: 1.697e+11 ph/s  
Cryojet Status: undefined  
Beamline Token:

01.02.13 12:02 Beamline Development, 400mA Top-up  
01.02.13 12:02 Problem fixed: accumulation started  
01.02.13 11:24 no beam for min. 0.5 hour

**Start** **Abort**

**Alignment Control**

**Camera Zoom**  
Low High

**Illumination**

Lamp  up

**Focus**

**Omega (°)**  
0.144 0°  
-10° +10°  
-45° +45°  
-90° +90°  
-180° +180°  
5 - +

**Sample Movement (μm)**

**Bookmarks**

**Label**

**Screening Collection Advanced**

Total Range (°): 720  
Wedge (°): 10  
Method: Inverse Beam

label	Energy (eV)
pk	12666
infl	12663
rm	12700

**Add Energy** **Delete All**

This will carry out a data collection on the \*first energy\* of the list. The \*total range\* is split in \*wedges\* and each \*wedge\* of data is collected on the \*direct\* and \*inverse\* wedge i.e. angle + 180 degrees.

**Start** **Abort**

# 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},

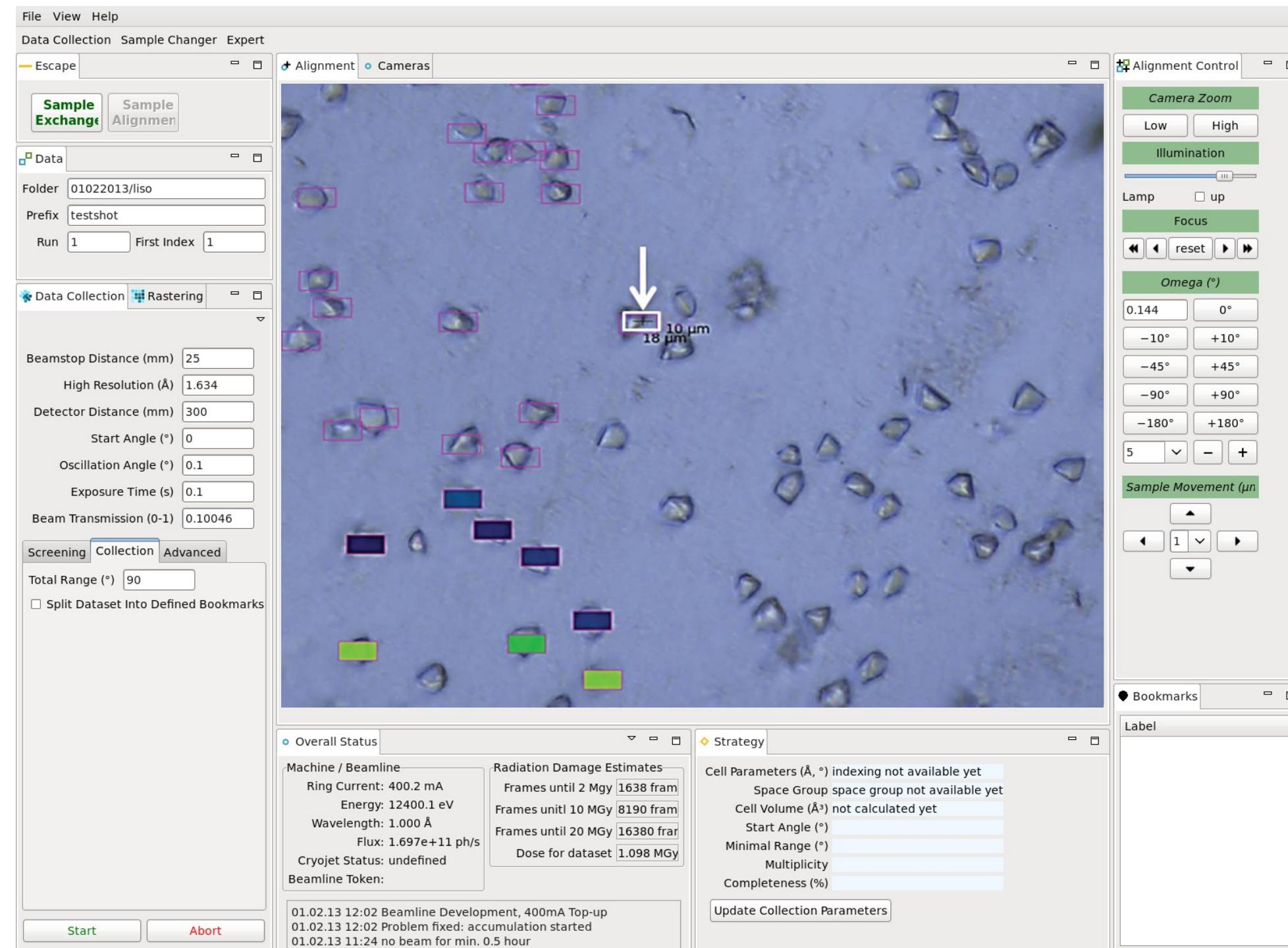
{
'energy': 11111.0,
'first_index': 451,
'folder': u'test/11111eV',
'num_frames': 450,
'prefix': u'testshot_11111eV',
'run': 1,
'start_angle': 45.0},

{
'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': 45.0},

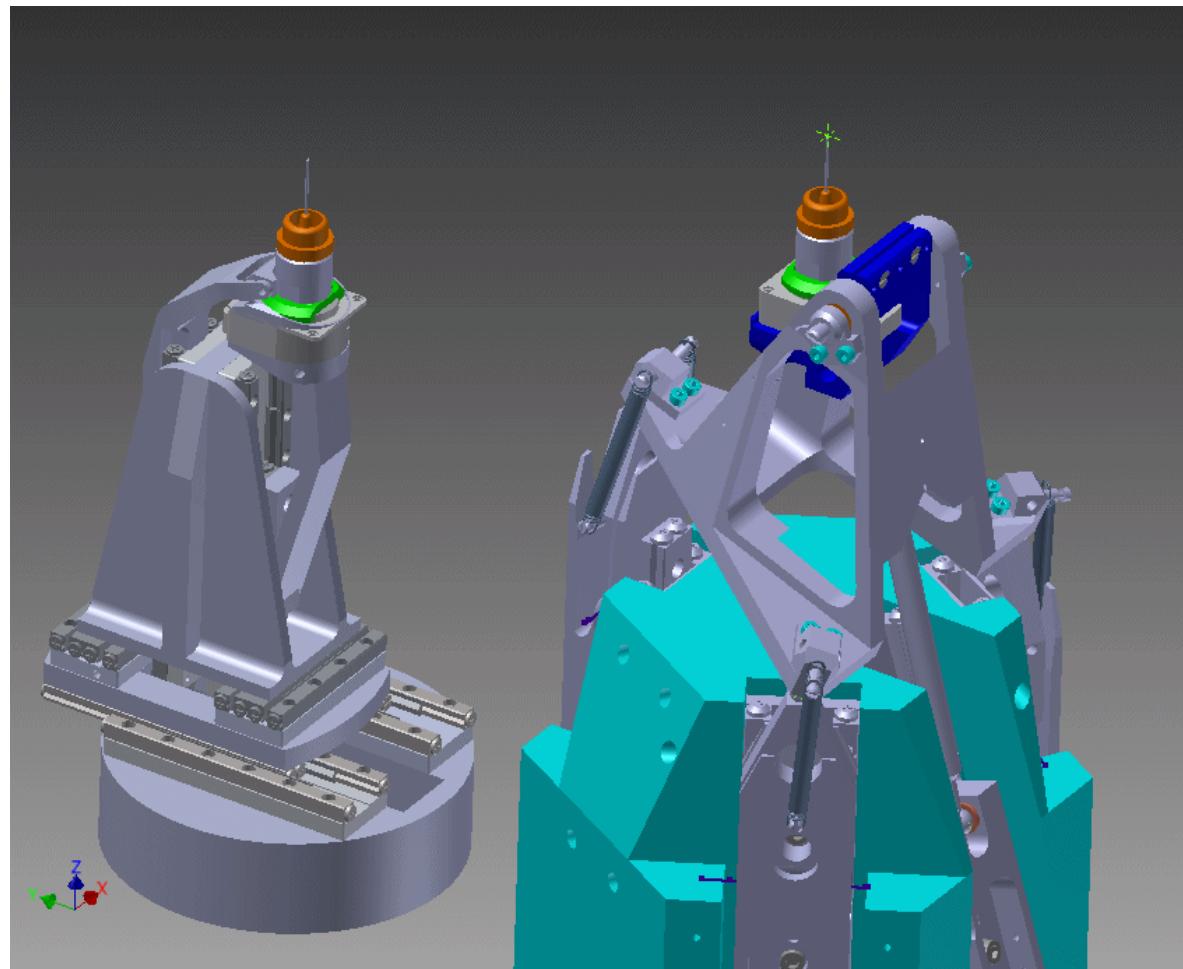
{
'energy': 8888.0,
'first_index': 451,
'folder': u'test/8888eV',
'num_frames': 450,
'prefix': u'testshot_8888eV_inv',
'run': 1,
'start_angle': 225.0}
```

# In situ minisets



# Sample Movers: multi-axis

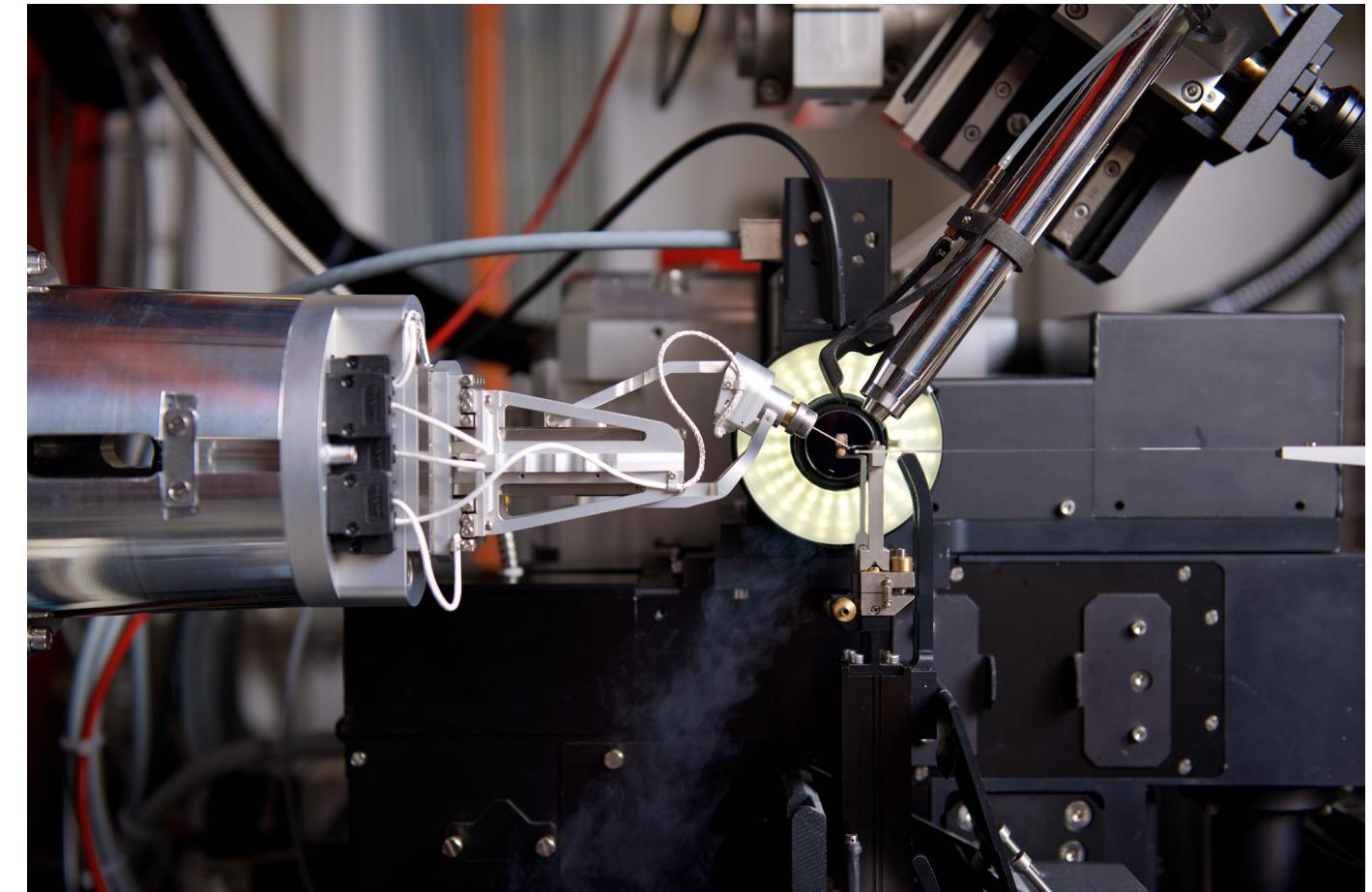
SmarGon



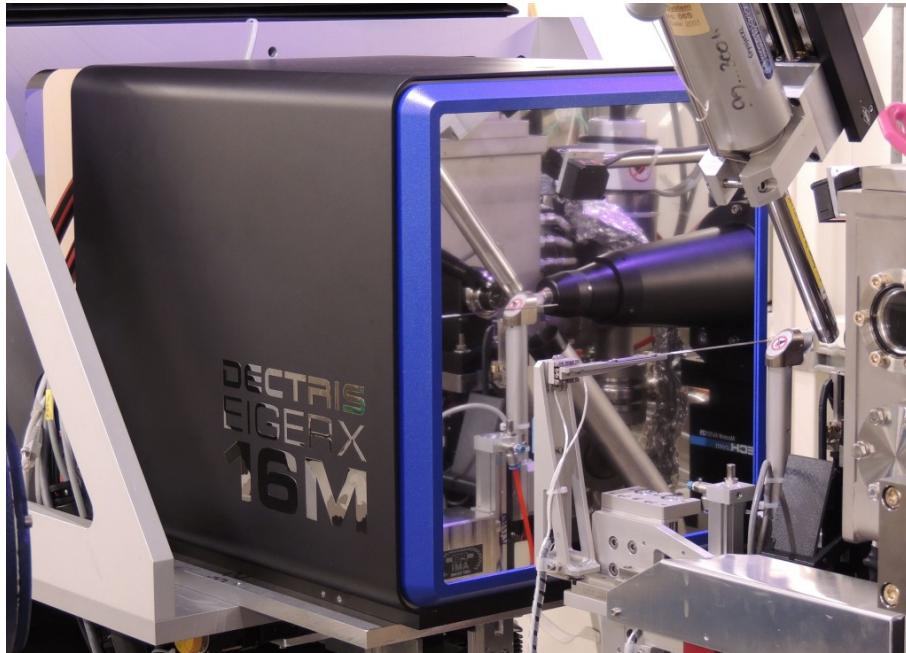
DeltaTau C.S. Orchestra C.S.  
5 μm SoC

PRIGo

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...



The End