

Progress towards connecting Global Phasing's workflow with MXCuBE

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MXCuBE meeting, Grenoble
January 2017

Contents

- Preamble
- Workflow architecture and MXCuBE connection
- Workflow demonstration

Introducing myself

- Coming from NMR, CCPN project
 - Data models and standards
 - Python application development
 - Software integration
 - Structural biology
- I am not a crystallographer
 - but I can learn.
 - Please be patient

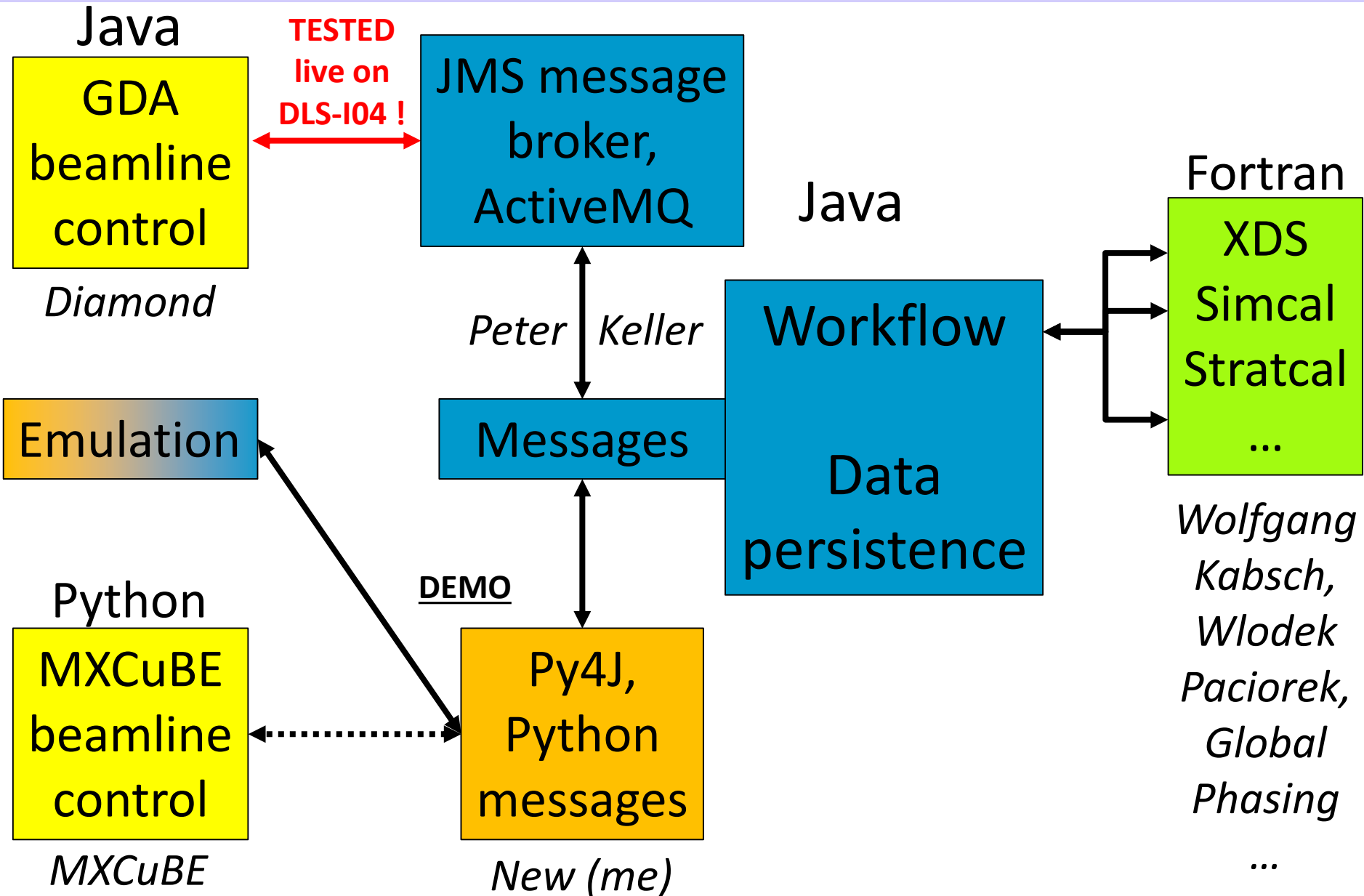
Contents

- Preamble
- **Workflow architecture
and MXCuBE connection**
- Workflow demonstration

Workflow operation

- Drives the beamline, data collection and (eventually) processing
- Beamline-independent core; messages using Abstract Beamline Interface
- Works through beamline control system
- Input, instructions and output through beamline user interface (or emulator)

Architecture



MXCuBE messaging

- Synchronous RPC calls from workflow
 - Beamline side py4j server
 - Java message objects
 - Python access via py4j
 - Conversion to pure Python message objects matching **Abstract Beamline Interface**
 - Self-contained, beamline-independent, can be replaced
- Messages trigger processMessage calls
 - Hook for beamline emulator, or beamline control
 - Intended to hook into MXCuBE queue

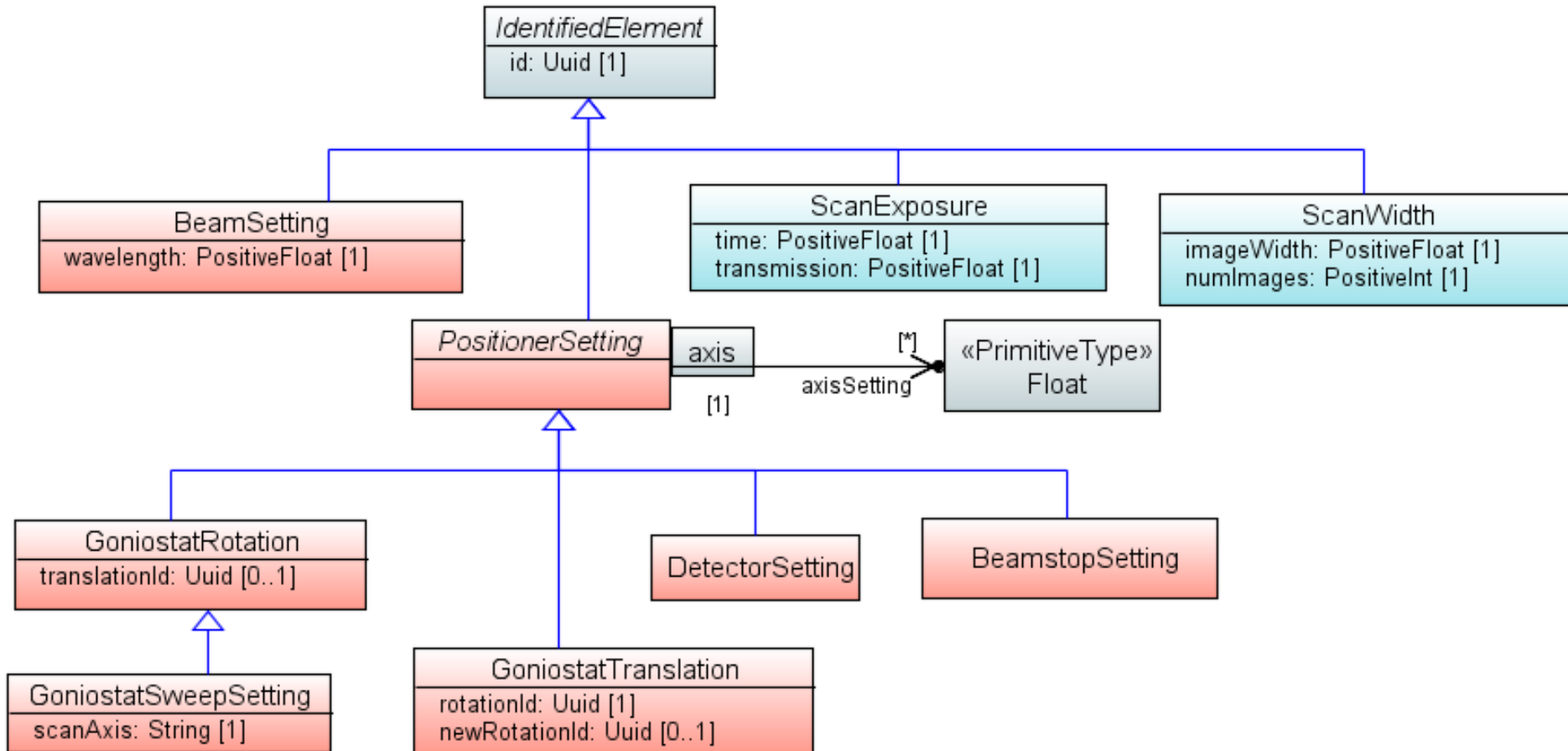
Messages from Workflow

- RequestConfiguration
- RequestCentring
- ChooseLattice
- GeometricStrategy (requests re-centring)
- CollectionProposal (requests data)
- Information messages:
 - SubprocessStarted
 - SubprocessStopped
 - Text (for echoing)
- Workflow Ready / Aborted / Completed / Failed

Messages to Workflow

- ConfigurationData
- PriorInformation (Sample initial data)
- SampleCentred
- SelectedLattice
- CollectionDone
- BeamlineAbort
- CentringDone (for calibration workflow)

Instrument Setting UML



Future issues

- Messaging protocol
 - Synchronous or asynchronous?
 - Is py4J OK?
 - XML-RPC server?
- Handshaking and control
 - Who triggers whom?
 - Processes, aborts, and restarts
- User interface
 - Need for changes or dedicated modules?
- Calibration and configuration
 - High standard required
 - Bespoke calibration workflows

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- **Workflow demonstration**

Demonstration

- I show running demo, interspersed with screenshots from live DLS-I04 test
- Workflow program runs in full production mode
- Client-server communication fully functional
- Beamline control system (BCS) is emulated by a plug-in replacement (mock-BCS)
- Mock-BCS runs as separate server process

Beamline emulation

- Mock-BCS based on
 - Configuration files
 - Sample description files
 - Dummy centring values
 - User input
 - Copies of pre-acquired characterisation images
- Full emulation (existing, not demonstrated)
 - Images calculated from structure model, mosaicity value, specific crystal orientation, ...

Workflow *demo* 1

- Start mock-BCS and workflow
- Load sample information and parameters
- Centre sample

DLS-I04 *live* - image 1

Applications Places System Fri 30 Sep, 17:24

Beamline I04 - Tel: +44 1235 778679 (Out of hours: +44 1215 778787) - GDA - B 56 0

File Edit Run Window Help Messages

Baton: ● Health: ● ● Panic Stop

Hutch Control: Prepare for Access

Current Sample: Lysozyme_2 (H36 S2) Barcode: NR

Sample Robot: Robot Options Robot Status: idle

Energy: 12658.0 eV

Wavelength: 0.97950 Angstro

Detector Distance: 500.00 mm

Flux: 0.00 photon/s

Aperture: 200µm

Machine: Ring Current: 300.25 mA

Refill: 346 s

ID Gap: 5.3449 mm

Monitoring: Beamline: idle

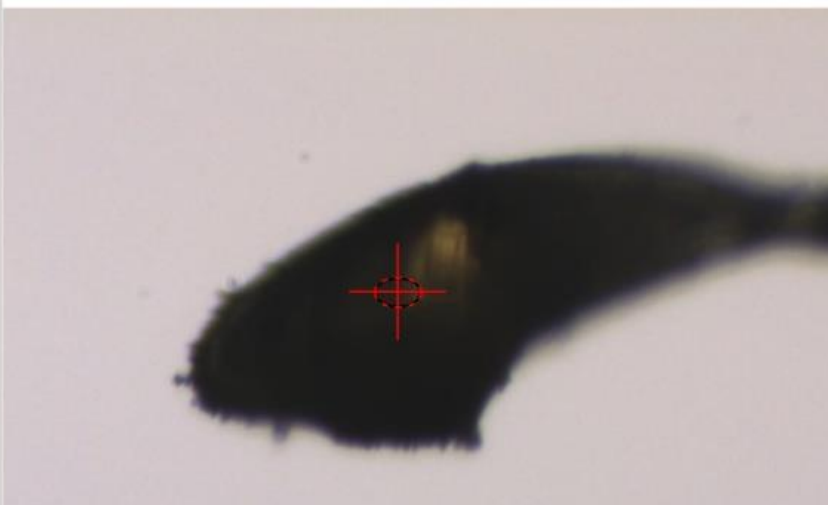
Script:

Sample Control: idle

User feedback: Send feedback

ISPyB Samples Alignment Grid Scan Grid Scan Results Fluorescence Data Collection Line Scan Tools User Options Reset Layout

OAV View Recentre: Centring complete



Camera Control: Beam Visualisation

Snapshot Backlight

Zoom: 7.5

Rotation:

Omega: 103.866 deg Kappa: 21.758 deg

Move to zero Move to zero

-90 +90 - + 10.0 deg

-180 +180 Phi: 131.641 deg

- + Move to zero

Size: 10.0 deg - + 10.0 deg

Translation:

Nudge: Readbacks

X: -1217.9 micron

Y: -191.8 micron

Z: -101.5 micron

Data Collection Settings Strategy Calculation Screening

Abort workflow

Initiate Completed Aborted

Sample Name: Lysozyme_2

ID: 2e9507ad-9bb4-4a4a-98fa-a1d253d254ca

Wavelength Selection

I know sample contains anomalous scatterer(s)

Wavelength (Å)	Role
0.97949	peak
0.97951	peak

I know which wavelength(s) to collect data for

Lattice information

Extract automatically

MTZ file:

Enter manually

Crystal system: Don't know

Space group:

Unit cell: a b c

Data Collection Table Input

Visit Folder: /dls/i04/data/2016/nt14493-31

Default Folder: \${proteinacronym}/\${samplename}

Default Prefix: \${samplename}

Folder	Prefix	Holder	Position	Omega Start (°)	Omega Oscillatio (°)	Omega Delta (°)	Kappa (°)	Phi (°)	Number of Images	Time per Image (s)	Maximum Resolutio (Å)	Distance (mm)	Wavelength (Å)	Energy (eV)	Transmission (%)	Beamstop position	Run Number	First Image Number	Comment
Lysozyme_2/stratcal	stratcal_gen_G0B0			193.87	0.100	0.00	21.758	131.640	900	0.100	1.5970	291.0	0.97949	12658.0	5.000000	Low Res.	2	1	x=-1.2179000000000004;y

Setting the workflow's initial parameters

Workflow *demo 2*

- Collect characterisation data
- Run indexing (XDS, COLSPOT, IDXREF)
- Select indexing solution

DLS-I04 *live* - image 2

Applications Places System Fri 30 Sep, 17:27

Beamline: I04 - Tel: +44 1235 778679 | Out of hours: +44 1235 778787 | GDA: 8.56.0

File Edit Run Window Help Messages

Baton ● Health ● Panic Stop

Hutch Control: Prepare for Access

Current Sample: Lysozyme_2 (H36 S2) Barcode: NR

Sample Robot: Robot Options Robot Status idle

Energy: 12658.0 eV

Wavelength: 0.97950 Angstro

Detector Distance: 500.00 mm

Flux: 0.00 photon/s

Aperture: 200µm

Machine: Ring Current: 299.07 mA

Refill: 134 s

ID Gap: 5.3448 mm

Monitoring: Beamline: idle

Script:

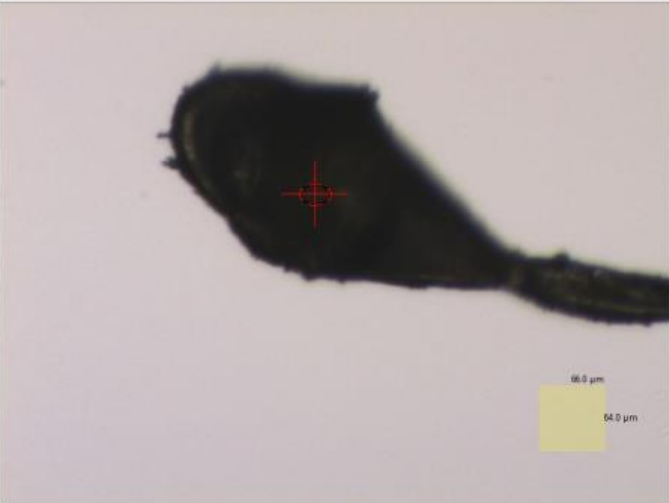
Sample Control: idle

User feedback: Send feedback

ISPyB Samples Alignment Grid Scan Grid Scan Results Fluorescence **Data Collection** Line Scan Tools User Options Reset Layout

OAV View Data Collection Settings Strategy Calculation Screening

Recentre Centring complete ● Aperture ■ Beam Scale ○ Focal Spot □ Slit Gap



Camera Control: Snapshot Beam Visualisation

Zoom: 7.5 Backlight

Rotation: Omega: 0.000 deg Kappa: -0.000 deg

Move to zero Move to zero

-90 +90 - + 10.0 deg

-180 +180 Phi 0.000 deg

- + Move to zero

Size: 10.0 deg - + 10.0 deg

Translation: Nudge Readbacks

X: -1233.1 micron

Y: -24.1 micron

Z: 210.8 micron

Abort workflow

Initiate Completed Aborted Running

GDA

ASTRA

XDS

ASTRA

* LATTI CHAR	BRAV LATTI	QUALIT OF FIT	UNIT a	CELL b	CONST c	(ANGST alpha	AND beta	DEG gamma
* 31	aP	6.0	37.3	78.9	79.0	89.8	89.9	89.8
* 44	aP	1.7	37.3	78.9	79.0	90.2	89.9	90.2
* 20	mC	3.5	111.9	111.5	37.3	90.1	90.2	90.0
* 35	mP	7.8	78.9	37.3	79.0	89.9	90.2	90.2
* 23	oC	8.5	111.5	111.9	37.3	89.8	90.1	90.0
* 25	mC	8.5	111.5	111.9	37.3	89.8	90.1	90.0
* 34	mP	11.3	37.3	79.0	78.9	90.2	90.2	89.9
* 33	mP	12.0	37.3	79.0	78.9	90.2	90.2	89.9
* 32	oP	15.8	37.3	78.9	79.0	90.2	89.9	90.2
* 21	tP	16.5	78.9	79.0	37.3	89.9	90.2	90.2
39	mC	248.8	162.1	37.3	79.0	89.9	90.2	76.9
37	mC	249.5	162.1	37.3	79.0	89.9	90.2	76.9
29	mC	252.6	37.3	162.1	79.0	89.8	90.1	76.9
28	mC	253.3	37.3	162.1	79.0	89.8	90.1	76.9
38	oC	256.8	37.3	162.1	79.0	89.8	89.9	103.1
36	oC	257.5	37.3	162.1	79.0	89.8	89.9	103.1
27	mC	493.8	162.1	37.3	111.5	89.9	133.4	76.9
19	oI	494.5	37.3	111.5	117.8	90.0	71.8	89.9
26	oF	610.8	37.3	162.1	162.2	86.8	103.2	103.1
18	tI	611.5	111.5	117.8	37.3	71.8	90.1	90.0
1	cF	999.0	117.6	117.5	117.8	95.7	95.7	143.0
2	hR	999.0	87.3	87.2	118.1	118.2	61.9	100.6
3	cP	999.0	37.3	79.0	78.9	90.2	90.2	89.9
5	cI	999.0	87.2	87.4	111.5	50.4	50.3	79.7
4	hR	999.0	87.3	87.5	117.5	117.9	61.9	100.4
6	tI	999.0	111.5	87.2	87.4	79.7	50.4	50.3
7	tI	999.0	87.3	87.4	111.5	50.4	50.3	76.7

Select lattice

Data Collection Table Input

Visit Folder: /dls/i04/data/2016/mt14493-31 Default Folder: {proteinacronym}/{samplename} Default Prefix: {samplename} Run All Run Selected

Row Sel.	Sample ID	Code	Folder	Prefix	Holder	Position	Omega Start (°)	Omega Oscillatio (°)	Omega Delta (°)	Kappa (°)	Phi (°)	Number of Images	Time per Image (s)	Max Res (Å)
	Lysozyme_2		Lysozyme_2/stratca	InitialCharacterisatic	36	2	0.00	0.100	0.00	0.000	0.000	12	0.100	1.5
	Lysozyme_2		Lysozyme_2/stratca	InitialCharacterisatic	36	2	45.00	0.100	0.00	0.000	0.000	12	0.100	1.5
	Lysozyme_2		Lysozyme_2/stratca	InitialCharacterisatic	36	2	90.00	0.100	0.00	0.000	0.000	12	0.100	1.5

qny31541 Baton held No Scan running No Script running Queue - waiting

Choosing an indexing solution

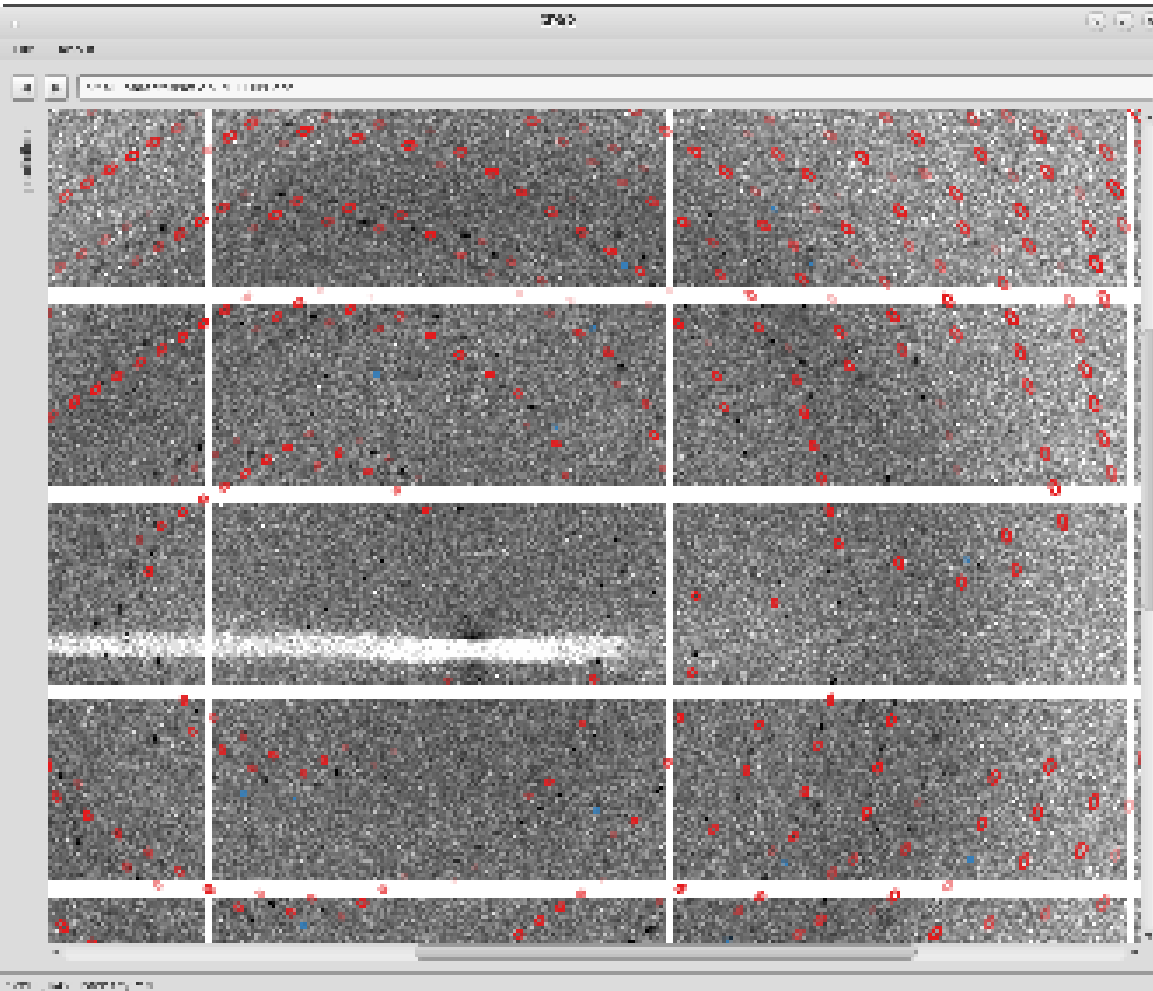
Workflow *demo* 3

- Calculate spot predictions from indexing solution for characterisation images (XDS, `simcal_predict`)
- User check of indexing solution (GPX2)

DLS-I04 *live* - image 3

GPX2 display of characterisation images

The spots used for indexing (faint blue crosses) come from the SPOTS.XDS file. Since these characterisation images are fine-sliced (0.1°) the spots are all partial, so that many of their blue crosses will be found on adjacent images.



This example shows some mismatch between predictions (red ellipses) and measured spots, probably due to a lack of up-to-date calibration data for the goniostat.

Workflow *demo* 4

- Calculate acquisition strategy (stratcal)

DLS-I04 *live* - image 4

Applications Places System Fri 30 Sep, 17:27

Beamline I04 - Tel: +44 1235 778679 | Out of hours: +44 1235 778787 - GDA - B 56.0

File Edit Run Window Help Messages

Baton ● Health ● ● Panic Stop

Hutch Control: Prepare for Access

Current Sample: Lysozyme_2 (H36 S2) Barcode: NR

Sample Robot: Robot Options Robot Status: idle

Energy: 12658.0 eV

Wavelength: 0.97950 Angstrom

Detector Distance: 500.00 mm

Flux: 0.00 photons/s

Aperture: 200 μm

Machine: Ring Current: 299.01 mA

Refill: 126 s

ID Gap: 5.3449 mm

Monitoring: Beamline: idle

Script:

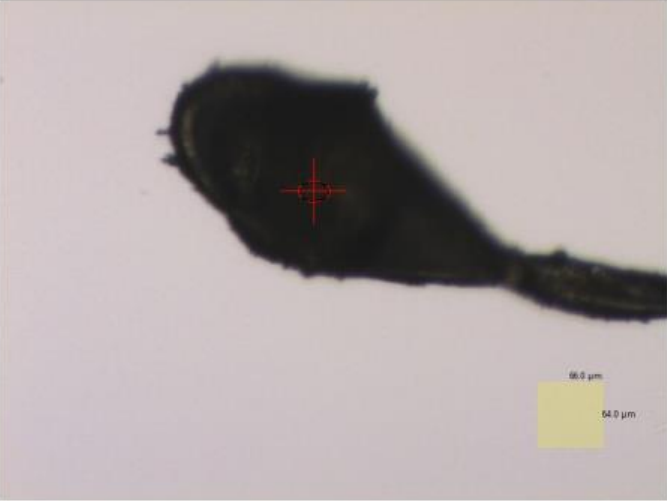
Sample Control: idle

User feedback: Send feedback

ISPyB Samples Alignment Grid Scan Grid Scan Results Fluorescence **Data Collection** Line Scan Tools User Options Reset Layout

OAV View Data Collection Settings Strategy Calculation Screening

Recentre Centring complete ● Aperture ■ Beam Scale ○ Focal Spot □ Slit Gap



Camera Control: Snapshot Beam Visualisation: Backlight

Zoom: 7.5

Rotation: Omega 0.000 deg Kappa -0.000 deg

Move to zero Move to zero

-90 +90 - + 10.0 deg

-180 +180 - + 10.0 deg

Phi 0.000 deg Move to zero

Size 10.0 deg - + 10.0 deg

Translation: Nudge Readbacks: X -1233.1 micron, Y -24.1 micron, Z 210.8 micron

Abort workflow

Initiate | Completed | Aborted | Running

GDA

ASTRA

XDS

ASTRA

XDS

simcal_predict

simcal_predict

stratcal

No collision or occlusion

Checking requested sweep: (1 3 1) 131.217 21.766 -165.677 -75.677
No collision or occlusion

Checking requested sweep: (3 1 1) 131.217 21.766 -75.677 14.323
No collision or occlusion

Checking requested sweep: (3 3 1) 131.217 21.766 -255.677 -165.677
No collision or occlusion

*** Select alignment pgp: First using k,m,n= 1 1 1

*** Analyse alignment: pgp ***

*** Select alignment pgp: Can't select first alignment!

Trial = 2

*** Analyse alignment: pgp ***

Checking requested sweep: (1 1 1) 131.217 21.766 -75.677 14.323
No collision or occlusion

Checking requested sweep: (1 3 1) 131.217 21.766 -255.677 -165.677
No collision or occlusion

Checking requested sweep: (3 1 1) 131.217 21.766 -165.677 -75.677
No collision or occlusion

Checking requested sweep: (3 3 1) 131.217 21.766 14.323 104.323
No collision or occlusion

Data Collection Table Input

Visit Folder /dls/i04/data/2016/nt14493-31 Default Folder \${proteinacronym}/\${samplename} Default Prefix \${samplename} ▶ Run All ▶ Run Selected

Row Sel.	Sample ID	Code	Folder	Prefix	Holder	Position	Omega Start (*)	Omega Oscillatio (*)	Omega Delta (*)	Kappa (*)	Phi (*)	Number of Images	Time per Image (s)	Max Res (Å)
	Lysozyme_2		Lysozyme_2/stratcal	InitialCharacterisatic	36	2	0.00	0.100	0.00	0.000	0.000	12	0.100	1.5
	Lysozyme_2		Lysozyme_2/stratcal	InitialCharacterisatic	36	2	45.00	0.100	0.00	0.000	0.000	12	0.100	1.5
	Lysozyme_2		Lysozyme_2/stratcal	InitialCharacterisatic	36	2	90.00	0.100	0.00	0.000	0.000	12	0.100	1.5

qny31541 Baton held No Scan running No Script running Queue - waiting

stratcal in mid-run

Workflow *demo* 5

- Check sample re-centring for each sweep of stratcal acquisition strategy

DLS-I04 *live* - image 5

The screenshot displays the DLS-I04 live control interface. At the top, the system status shows 'Applications Places System' and the date 'Fri 30 Sep, 17:21'. The main control area includes:

- Machine Parameters:** Energy 12658.0 eV, Wavelength 0.97950 Angstrom, Detector Distance 500.00 mm, Flux 0.00 photon/s, Aperture 200µm, Ring Current 301.16 mA, Refill 503 s, ID Gap 5.3449 mm.
- Monitoring:** Beamline: idle, Script: [empty], Sample Control: idle.
- User feedback:** Send feedback button.
- Current Sample:** Lysozyme_2 (H36 S2), Barcode NR.
- Sample Robot:** Robot Options, Robot Status: idle.

The central camera view shows a dark, circular crystal with a red crosshair. The zoom is set to 7.5. The rotation controls are set to Omega -166.134 deg and Kappa 21.758 deg. The translation controls show X: -1217.9 micron, Y: -214.7 micron, and Z: -107.2 micron. The beam size is 31.72 µm, and the lighting is set to Backlight Brightness 40% and Frontlight Brightness 0%.

On the right, the 'Data Collection Settings' panel shows a workflow table:

Initiate	Completed	Running
GDA		
ASTRA		
XDS		
ASTRA		
XDS		
simcal_predict		
simcal_predict		
stratcal		
ASTRA		

Below the table, the orientation is set to Phi=131.6° Kappa=21.8° and Omega: [-166.1...-76.1]°. The 'Degrees per image' is 0.1 and 'Images per wedge' is 100. A 'Collect as centred' button is visible.

At the bottom, the status bar shows 'qny31541', 'Baton held', 'No Scan running', 'No Script running', 'Queue - waiting', and 'Moving gonomega by 90.0'.

Centring the crystal for the strategy output by stratcal

Workflow *demo* 5

- Collect data
- Demo ends here

Where we are

- Workflow engine fully operational
 - Tested and working on live beamline (GDA/ASTRA, DLS-I04)
- Message transfer to Python fully operational
 - Running under demo
 - Current (prototype) implementation could be replaced
- Next step is connecting to MXCuBE queue

END