Incorporation of Global Phasing workflows in MXCuBE

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MXCuBE / ISPyB joint meeting
Trieste, September 2018

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Contents

- **Introduction**
- Workflows
- Status
- Live DEMO

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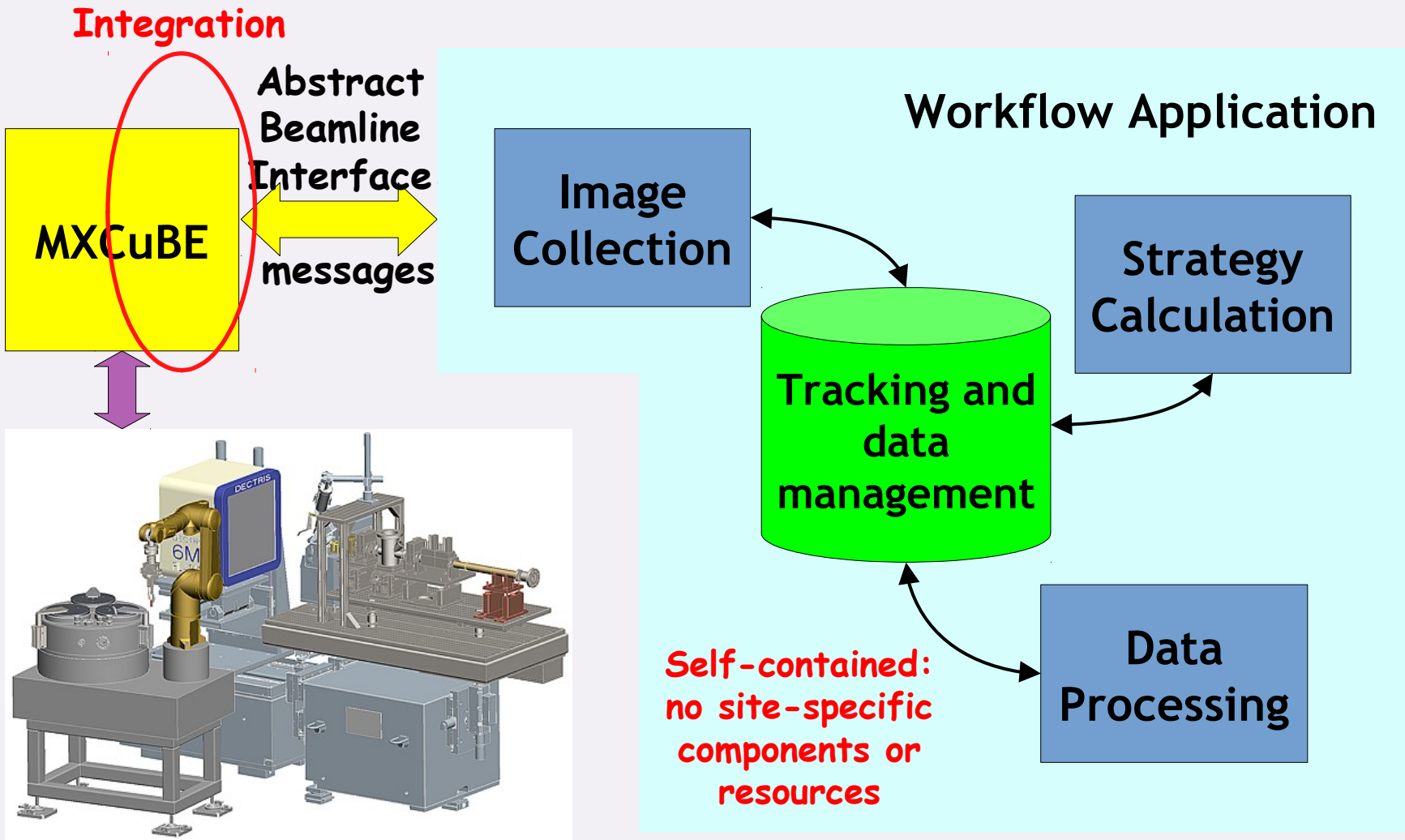
Driving a beamline as a third party



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Data collection workflow

- Optimal data collection strategy *While U Wait*
- Strategy determined in the workflow *outside* MXCuBE
- Requires multi-axis goniostat
- Requires precise translational and rotational calibrations
  - Calibration workflows provided
- Uses normal MXCuBE machinery, with additions

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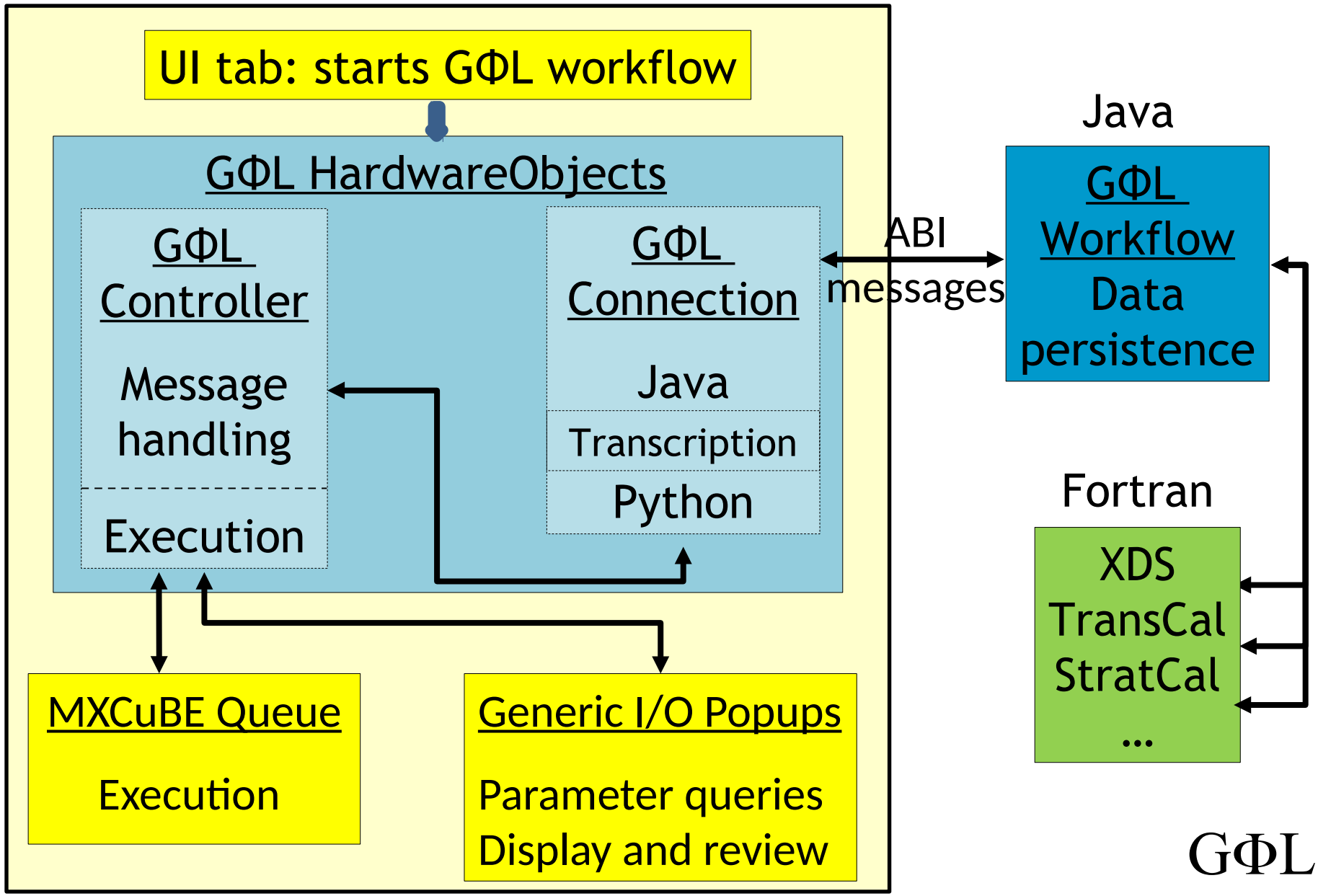
Integration architecture



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Data collection strategies

- Calculate strategy *after* characterisation step
  - Base strategy on indexing space group
  - Base alignment on known crystal orientation
- Multiple sweeps for completeness (e.g. for avoidance of empty cusps)
- Automatic re-centring after change of orientation
- Allowance for shadowing and collision avoidance

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Phasing data

- Align symmetry axis for optimal anomalous differences
  - Anomalous pairs on same image, with same scaling and radiation damage
- One or more wavelengths
- Automatic inverse-beam and wavelength interleaving (configurable)
- *Tested and working*

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Native data

- One or more sweeps, with alignment for completeness and balanced redundancy
- Now executes in mock mode
- Upcoming test at ESRF ID30B
  - *last ever in Qt3 branch*

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Translational calibration

- Optical calibration using fine-tip fibre
  - 30 centring points, in two stages
- Automatic re-centring after first stage
- ca. 5µm re-centring precision
- Keep sample centred between successive reorientations
- Manual sample centring under maximum zoom
- See example

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Re-centring example

Diffractometer calibration

- Uses images from high-symmetry crystal
  - Covers the detector surface
- Produces
  - accurate goniostat axis orientations
  - accurate detector origin,
    position and offsets for individual segments
- One multi-orientation data collection,
  slow processing (hours)

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Data collection example

- Crystal: Thaumatin, $P4_12_12$
- 0.1° per image
- Strategy:
  - A: 45° sweep, aligned with fourfold axis
  - B: 90° sweep, orthogonal to fourfold axis
  - C: 90° sweep, orthogonal to fourfold axis

    B,C inverse-beam, interleaved in 9° wedges

  - Acquired and processed (1.5Å)

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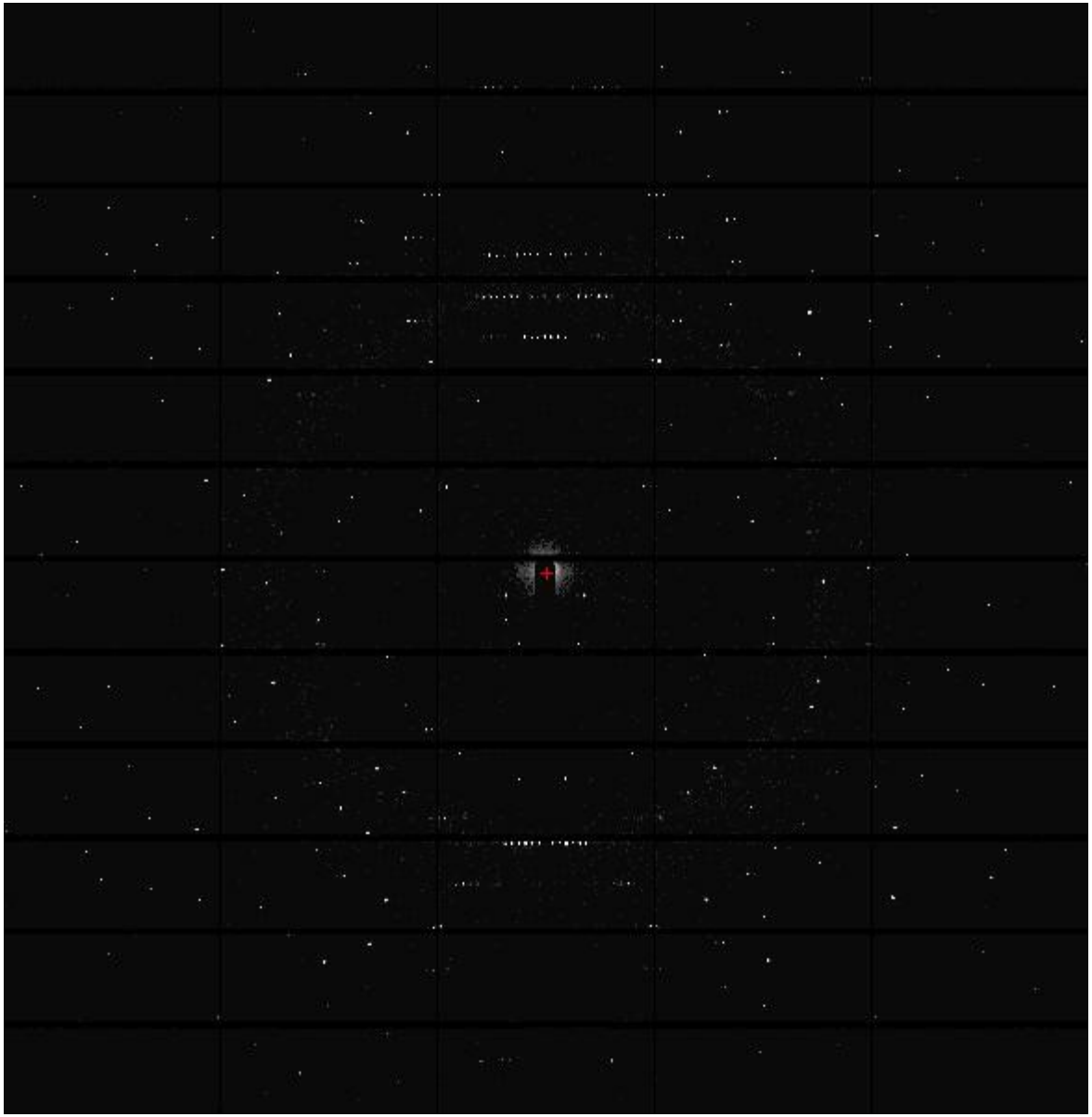
Axis-aligned image



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Testing over past year

- Two visits and five remote test sessions at ESRF ID30B
- Completed debugging and improved Qt3 version
- Successful execution of
  - Translational calibration
  - Diffractometer calibration
  - Single-wavelength, two-orientation data collection workflow
- Ported to master (Qt4) and further improved
  - Newer MXCuBE version much easier to work with

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Plans for coming year

- Test and install Qt4 version at multiple beamlines (ALBA, SOLEIL, more welcome)
- Make phasing strategy workflow available for use by early adopters
- Test native data strategies
- Extend integration to MXCuBE v3 interface
  Some help may be required

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Thanks to

- Andrew McCarthy, Antonia Beteva and Marcus Oscarsson for testing and assistance at the ESRF

- All the MXCuBE developers for help and collaboration
  - also for dockers, mock objects, and structured repositories

- My colleagues at Global Phasing.

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END

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