Connection and execution of GPhL workflows through MXCUBE
-
Status report and demonstration

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Global Phasing

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Contents

- **GΦL implementation and features**
- Status
- DEMO

Data collection workflow

- Getting the best possible data!
- Align unique axis; fill in cusp.
  Fall-back if optimal strategy not possible.
- Multiple orientations (ω, κ, φ) or (ω, χ, φ);
  Workflow-driven reorientation
- Strategies have built-in collision avoidance
  and anticipation of shadowing.
- Interleaving between different orientations,
  wavelengths, …
  - Automatically re-centre for each wedge
  - Calculating precise centrings
    from a single centring measurement

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Calibration Workflows

- Translational calibration
  - 6+24 centring steps at selected kappa, phi angles
  - Automatic centring after preliminary 6 steps
  - Automatic centring for all kappa, phi
    for use in other workflows

- Diffractometer calibration
  - 22*60deg acquisition with test sample
  - Precise calibration of diffractometer axes and detector

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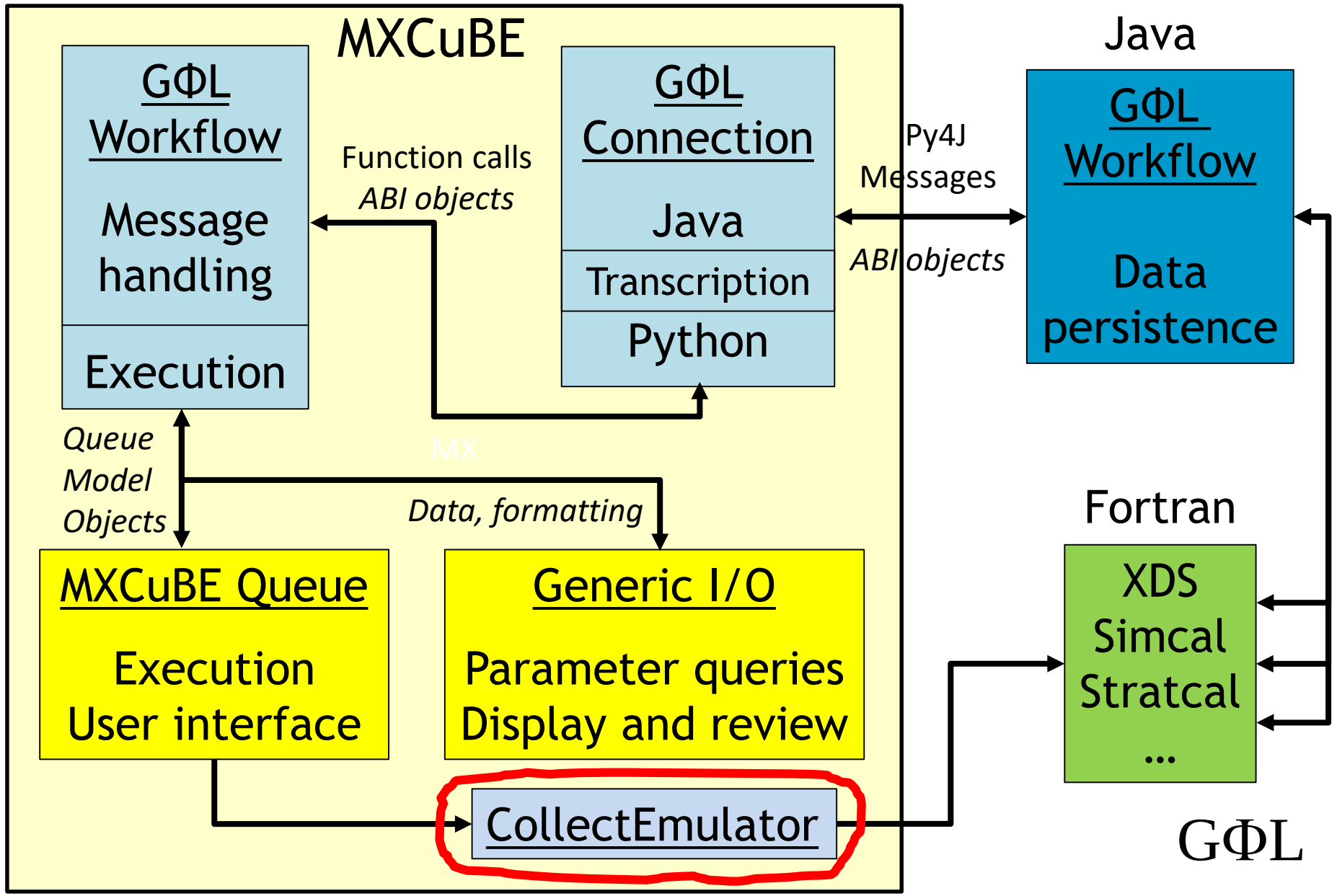
GΦL Workflow integration



Data collection emulation

- Simulates images
  - Input from MXCuBE collection queue
  - Test samples in SC-mockup. Required:
    - Crystal description (.nml format)
    - hkl-intensity file
- Fully integrated in MXCuBE
  - CollectEmulator, subclass of CollectMockup
  - Works off MXCuBE normal data structures
  - Uses data_collection_hook()
  - Calls GΦL *simcal* to generate images
  - Should work also for non-GΦL cases (TBT)

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Status

- Qt3/2.1 implementation
  - Tested live at ESRF-ID30B
  - Translational calibration works: 10µM precision
  - Diffractometer calibration: final bug found (?)
  - Data acquisition: final bug found (?)
    - *kappa, phi move commands were not executed by beamline software*
  - Will be abandoned for licensing reasons (?)

- Qt4/master implementation
  - Tested in mock/emulation mode only.

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Next steps

- Merge code into master
- Live test and complete Qt4 version
- Write and test mxcube3 / web version

- Wanted: collaborators

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END

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