The Abstract Beamline Interface in practice

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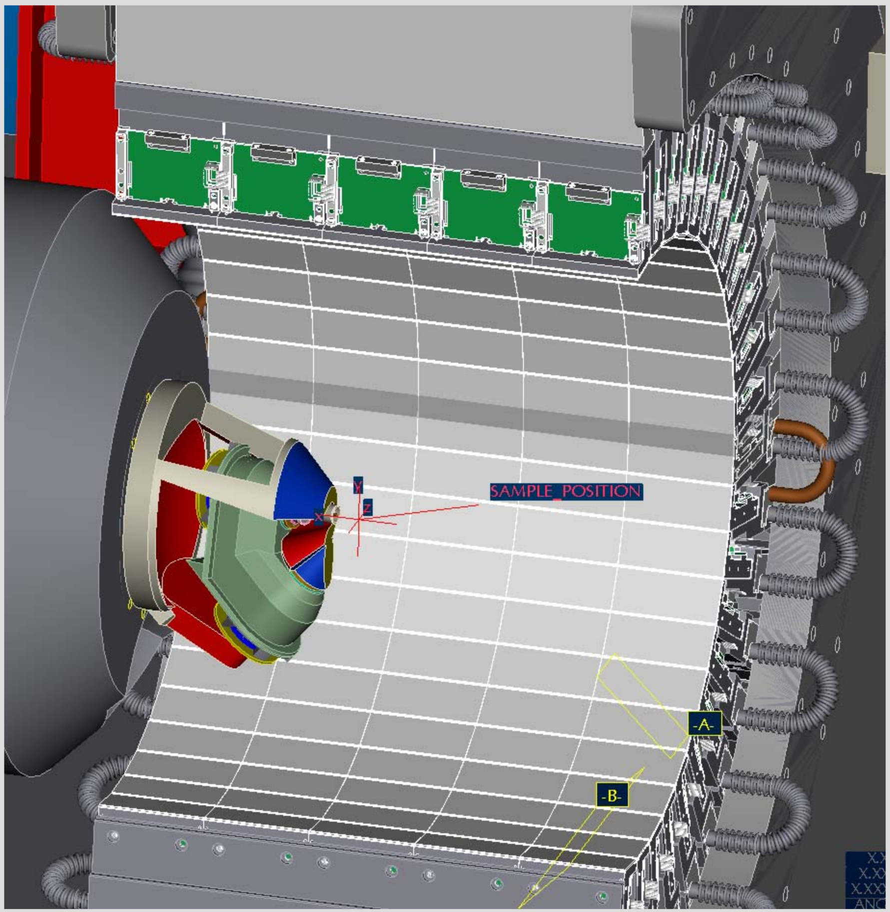
Overview

- Background
  - DLS-I23
  - Third-party protocols: the transferable workflow approach
- Changing priorities
- Calibration

GΦL

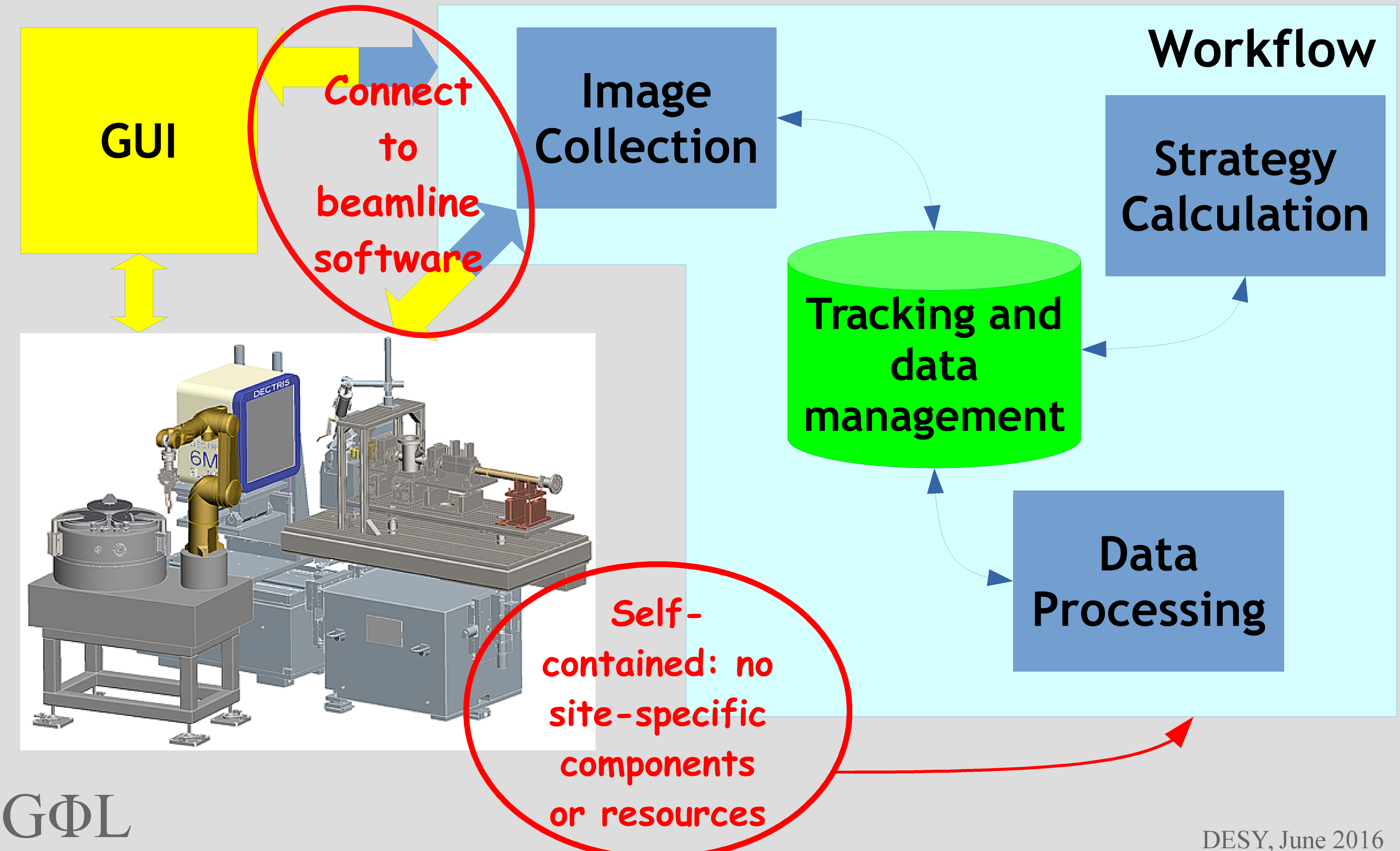
Challenges posed by the DLS-I23 beamline



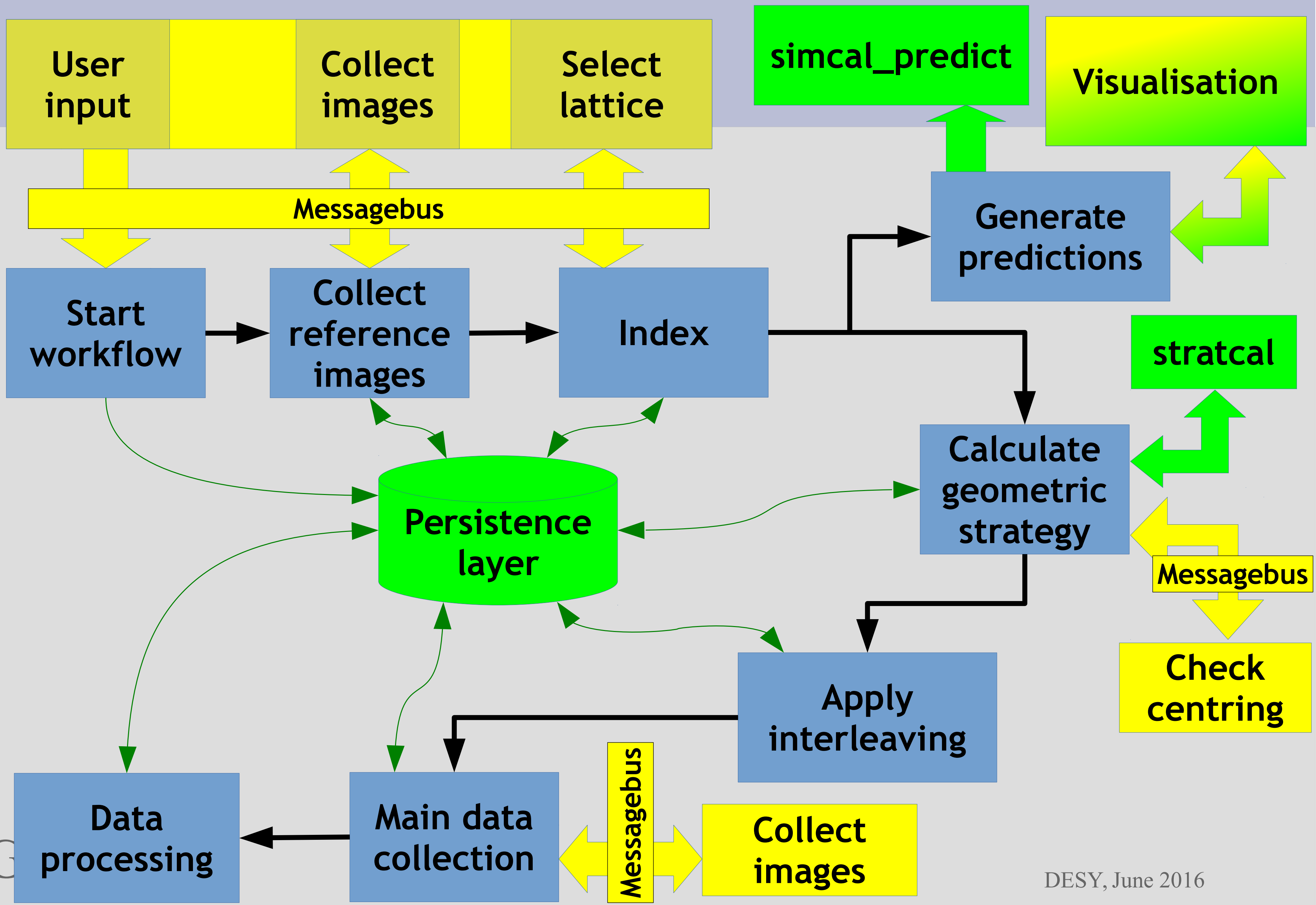
- Multiple orientations
  - Required by detector geometry
- Moving shadows
  - Cannot be realistically avoided
- Interleaving
  - Especially important for longer wavelengths
- Collisions

Particularly severe at I23, but can affect any beamline

Driving a beamline as a third party



Workflow with beamline



Workflow ↔ Beamline communication (1)

- Transferability is paramount
- Beamline-agnostic vocabulary
  - Restrict scope to data relevant to strategy calculation and data processing
- Connect to the Beamline Control System
  - No direct communication with beamline motors/devices
  - Use a communication technology that is supported by the BCS

Workflow ↔ Beamline communication (2)

- Abstract Beamline Interface
  - Definition of data exchanged between workflow and beamline
  - The current version was published on GitHub in November 2014
    - Originally proposed to the MXCuBE collaboration in June 2012
- Messaging protocol/technology:
  - DLS/GDA: Native Java serialisation of object graphs with JMS (Java Messaging Service) and Apache ActiveMQ
  - Future MXCuBE: XML-RPC (probably using Apache XML-RPC on the workflow side). Interaction with MXCuBE3 GUI: TBD.

Changing priorities (1)

- There have been delays in delivery and commissioning of some of the bespoke DLS-I23 instrumentation
- Decision: change focus to DLS-I04
  - a tunable, variable/micro focus beamline that is more conventional than I23:
    - Wavelength range: 0.71Å – 2.07Å
    - Mini-kappa goniostat
    - Pilatus 6M detector

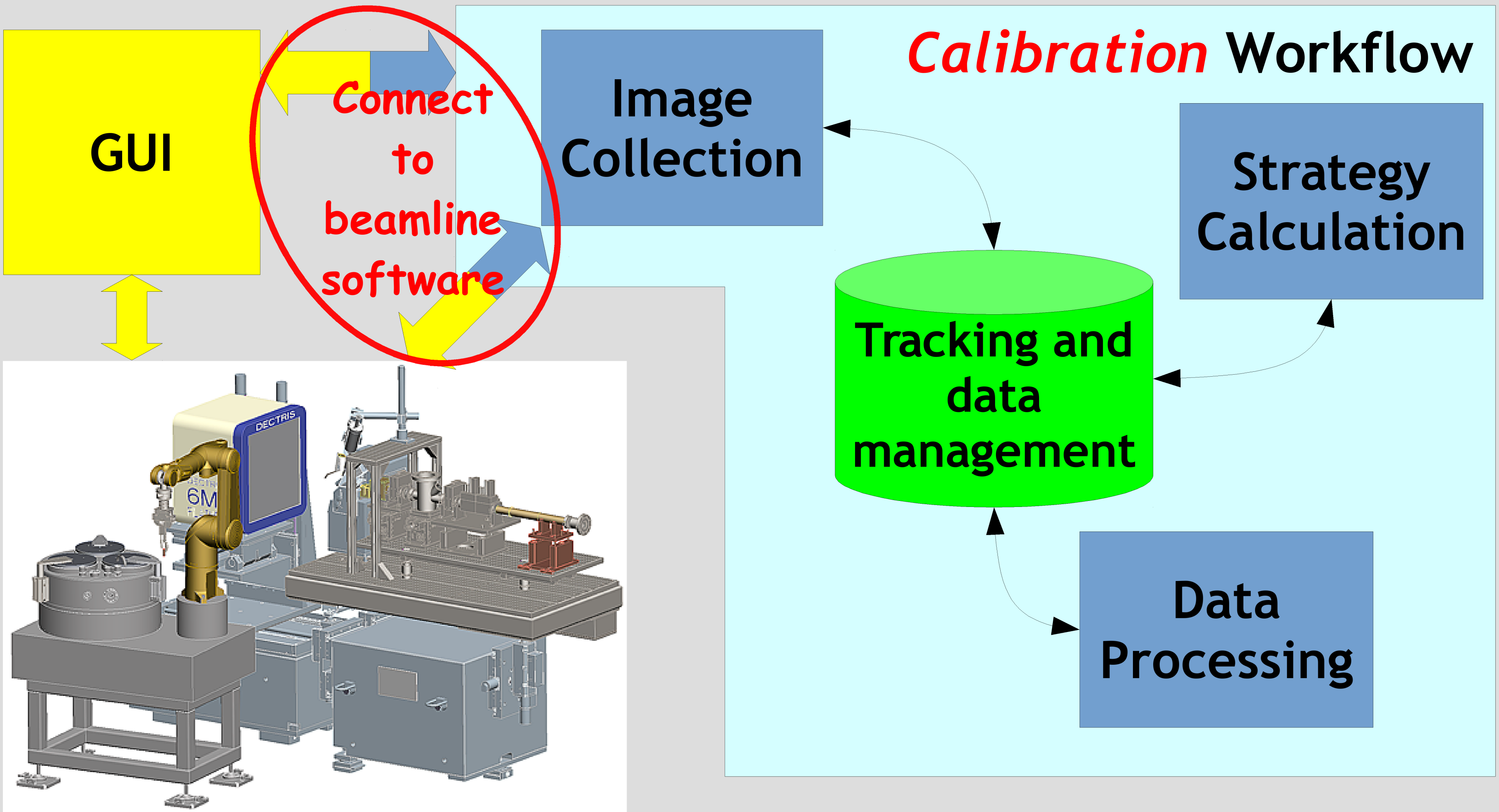
Changing priorities (2)

- DLS-I04 (unlike I23) is fully operational; this brings other issues forward:
  - technical: requirement for calibration data
  - hardware: real-world behaviour of the instrumentation
  - scientific: strategy determination for non-I23 hardware
  - software: readiness of workflow and Beamline Control System.
- Addressing these issues will help with:
  - deployment at non-DLS beamlines
  - application to strategies other than the phasing experiments that I23 was designed for

Beamline calibration

- Calculating and executing advanced strategies requires extensive, accurate beamline calibration data
  - Not available from standard beamline procedures
- The original ideas about driving MX experiments are being extended to calibration procedures:
  - translational (centring stage) calibration
    - optical
  - goniostat rotation axis and detector calibration
    - by diffraction

Driving a beamline as a third party



Workflow-driven calibration

- Aimed at beamline staff rather than users
- GΦL can provide the procedures that will produce the calibration data that GΦL applications require:
  - no need to “scavenge” existing data that may not be sufficient or appropriate
  - like MX experimental workflows, will be transferable to other beamlines
  - consistent, and of known provenance,
    - e.g. no surprise inconsistencies between MOSFLM and XDS-refined calibration results

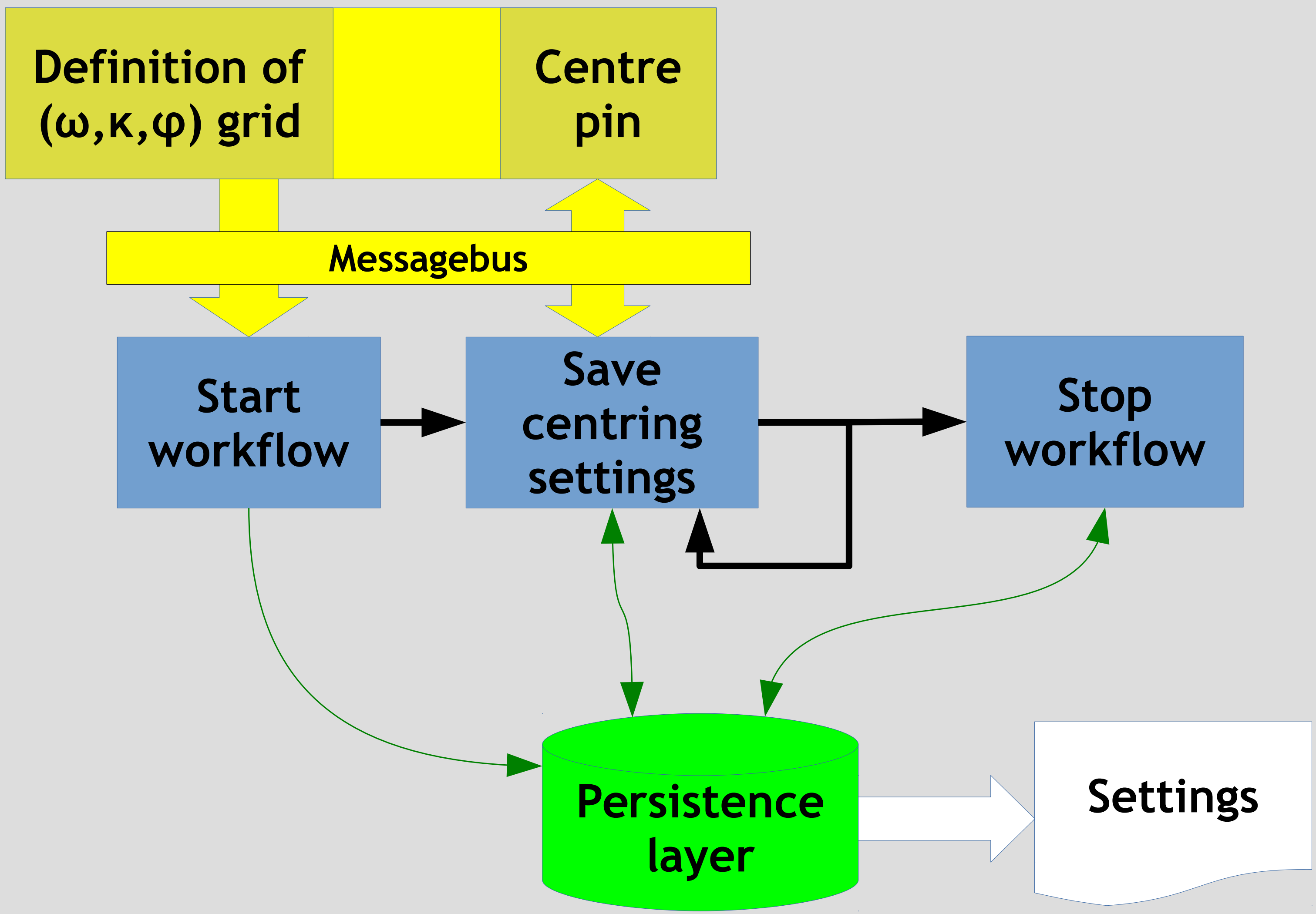
Translational calibration (1)

- Centring of the tip of a pin at many values of (ω,κ,φ)
  - optical procedure using OAV: no beam needed
- The initial attempt to calibrate the centring stage using* existing facilities on DLS-I04 was slow and painful
  - hundreds of data points needed
  - 27 data points per hour collected
  - * “subverting” might be a better description

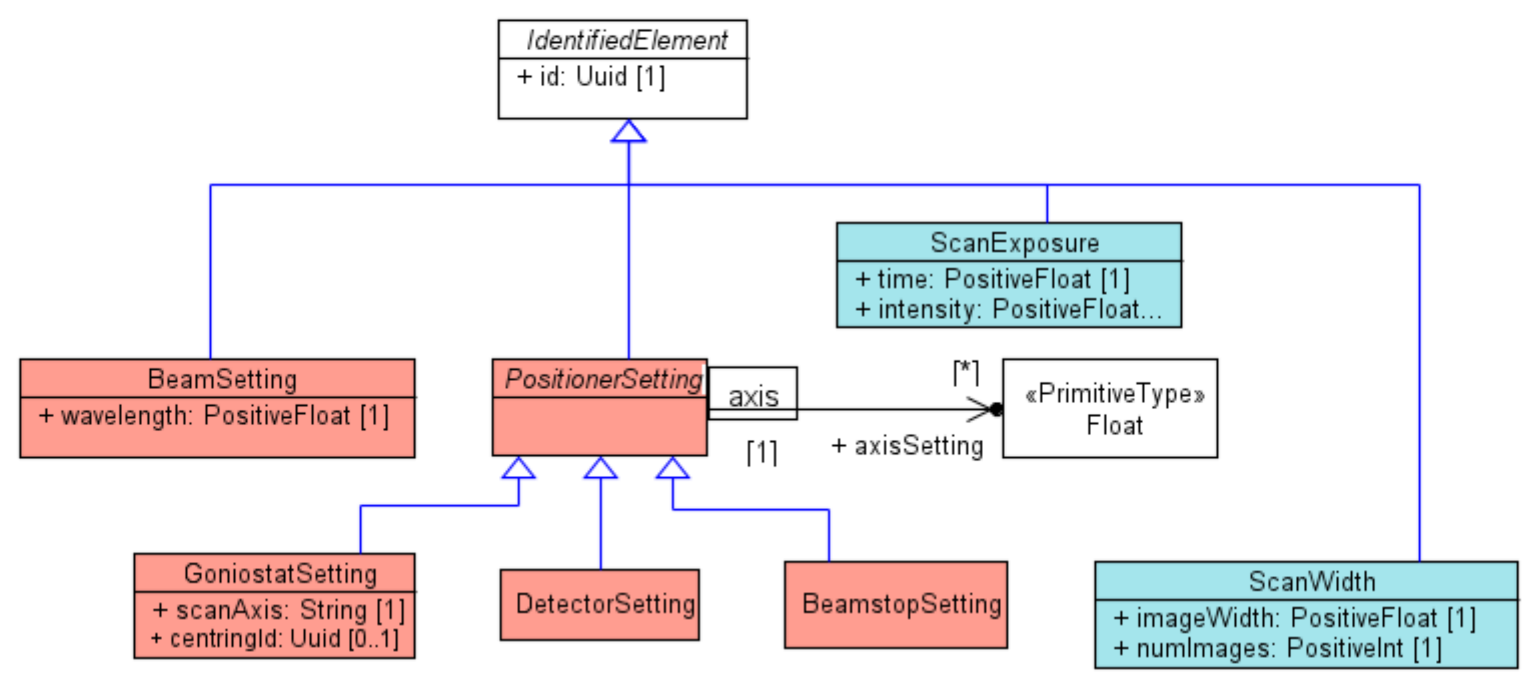
Translational calibration (2)

- We developed a workflow-based approach that enabled:
  - speed-up to 110 data points per hour
  - fully automatable by DLS, in principle
- Repeated by DLS staff without GΦL staff present
- Allowed verification of stratcal's functionality for anticipating re-centring settings between orientations

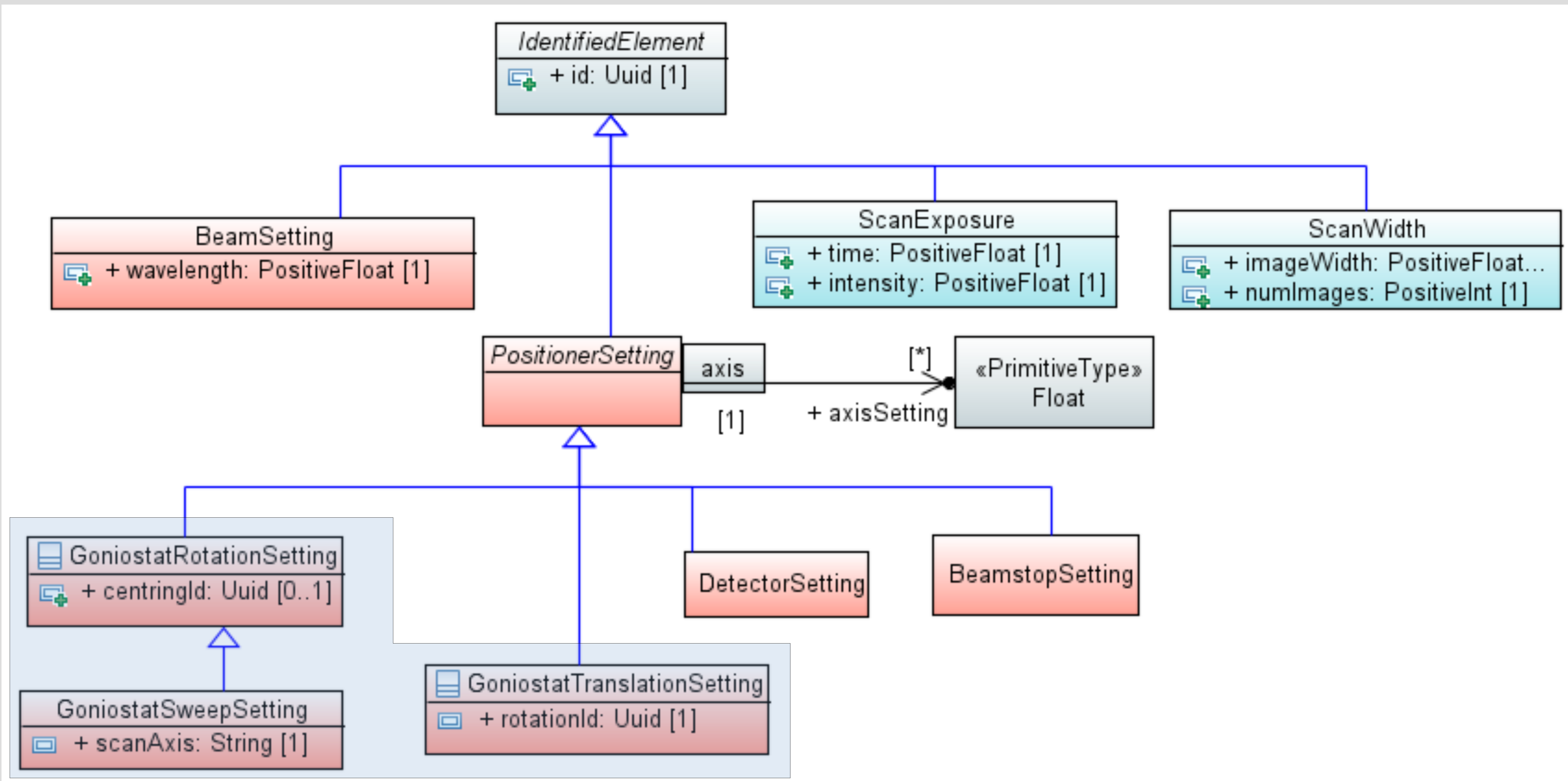
Centring stage calibration workflow



Centring stage calibration: Abstract Beamline Interface (before)



Centring stage calibration: Abstract Beamline Interface (after)



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Goniostat and detector calibration

- Diffraction-based procedure
  - collect data according to a particular protocol from a sample with specific characteristics
  - process images with the GΦL-developed XCALIBRA application
- In the future, will also be invokable from calibration workflows
  - no significant operational speed-up expected through workflow control in this case
  - essential to ensure consistency and provenance of the results, and control over processing

People involved

- GΦL: Gérard Bricogne, Claus Flensburg, Wlodek Paciorek, Clemens Vonrhein
- DLS: Jonathan Blakes, Ralf Flaig, David Hall, Pierpaolo Romano, Armin Wagner, Graeme Winter