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How to set up the GPhL workflow

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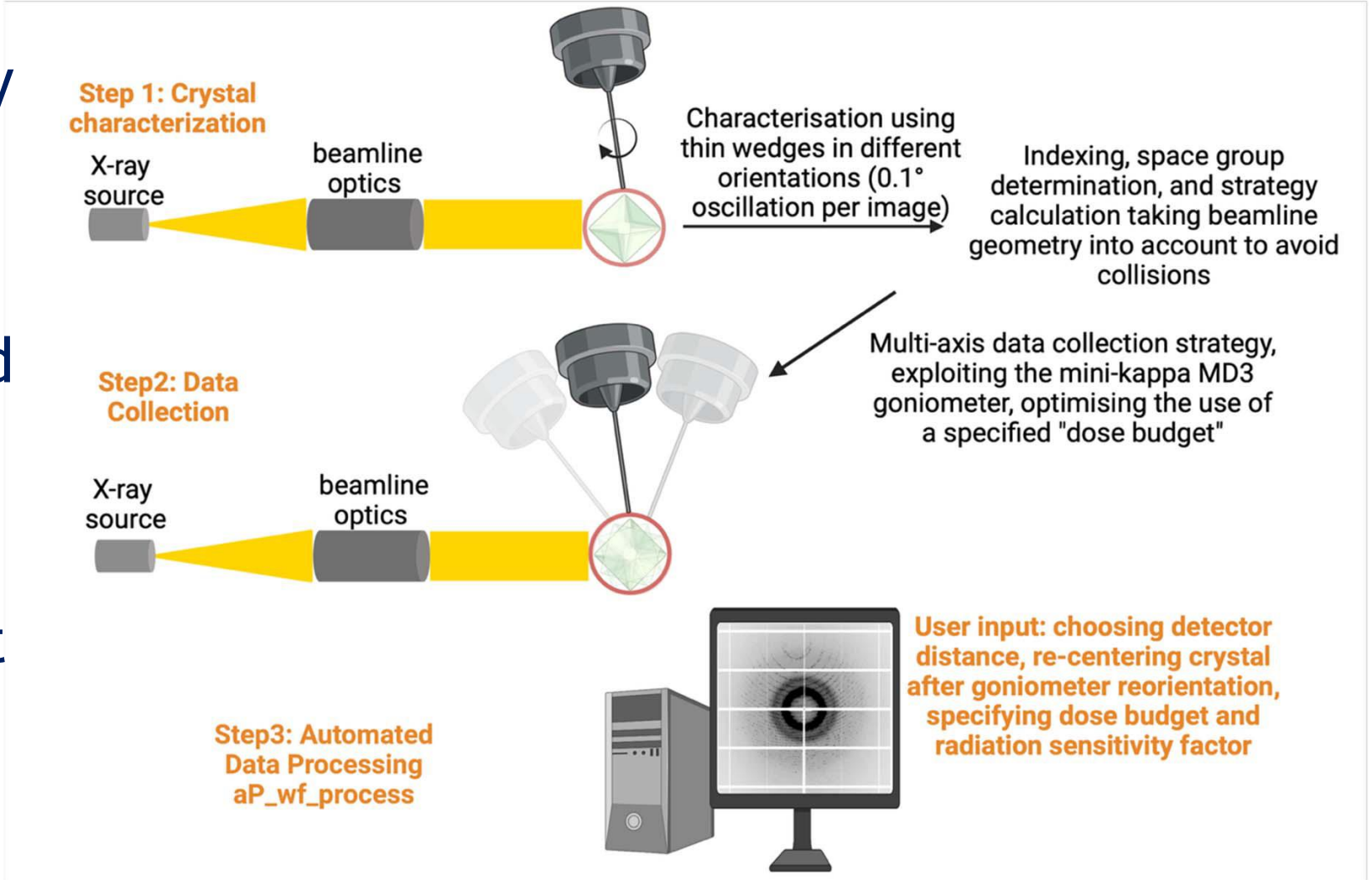
MXCuBE/ISPyB Meeting, HZB Berlin, 11 June 2026

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The Global Phasing workflow

- Acquiring high-quality experimental data routinely
- Manual or unattended
- What an experienced crystallographer who knows the instrument and the sample – and has time to think – would do



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Factors considered by the workflow

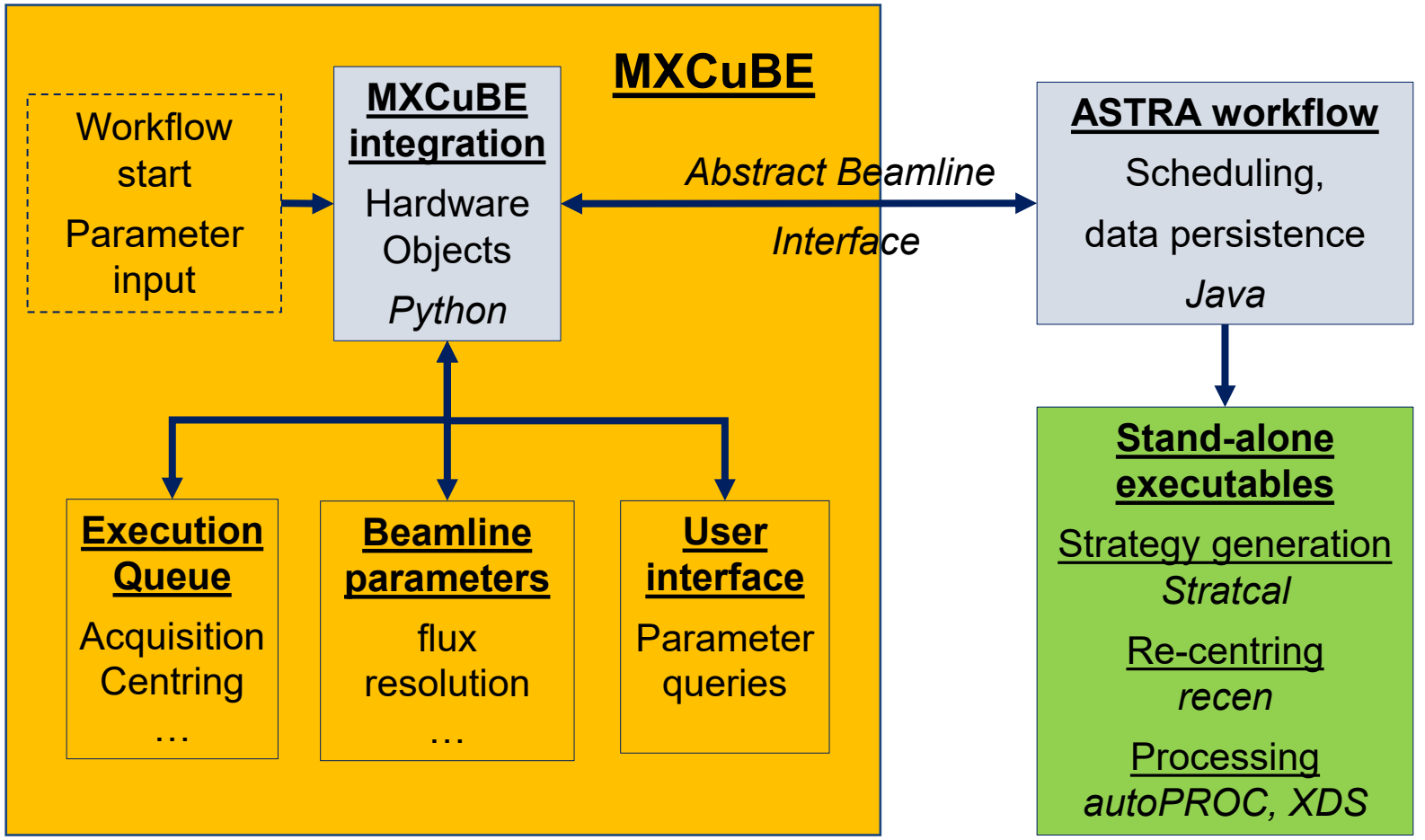
- Set transmission for optimal (resolution-dependent) dose budget
- ‘Basic’ variant
  - Short, avoiding very bad orientations (cusps) and parameter settings
- ‘Advanced’ variant
  - Longer, with high multiplicity and Lorentz-factor enhancement both spread as evenly as possible over all reflections
  - Use high kappa angles while avoiding goniostat shadows in the images
  - Set sweep widths for improved scaling and multiprocessor timing
  - For phasing, improve anomalous signal using inverse-beam and/or alignment of even-fold axes, and dispersive signal by energy interleaving

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Program structure

- The GPhL workflow is a stand-alone, BCS-independent application
- Integration to MXCuBE is via embedded GPhL hardware and queue model objects



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Requirements for GPhL workflow

- You need an up-to-date MXCuBE version, with either web or Qt interface
  - GPhL integration is built into MXCuBE, but versions must match
  - GPhL cannot support integration in multiple, diverging MXCuBE versions
- Support for multiple wedges at the same orientation is needed for the characterisation strategy (or for interleaved phasing)
  - This can be non-trivial for HDF5 files
- Currently only mini-kappa goniostats are supported – Smargon is on the TODO list
- The workflow is licensed for non-profit users or GPhL Consortium members

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Dependencies

- The workflow is a stand-alone installation, with its own conda environment and its own Python
- Communication between workflow and MXCuBE side uses a BCS-independent *Abstract Beamline Interface*
  - The messaging library Py4J is the main dependency on the MXCuBE side
  - Upgrade to another library might eventually be possible
- Support for other beamline control systems might in theory become possible
  - This would require writing a new BCS-side integration code to receive and act upon the ABI messages

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Requirements for unattended operation

- Functional automated (X-ray) centring
  - For crystal finding and initial centring
  - High-quality and fast re-centring desirable for multi-sweep experiments
- Integration with your unattended-runner program
  - The GPhL workflow can be started with a single MXCuBE function call
  - You need to organise how to set defaults and provide input parameters
- Accommodation between unattended-runner and GPhL workflow is possible
  - At MASSIF-1 characterisation and initial XDS run are done by MXPress

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Detailed beamline description

- The GPhL workflow requires more detailed beamline configuration
  - This is kept in GPhL-specific configuration files
- Rotation and translation axis directions must be calibrated and kept up to date, particularly for effective recentring
  - GPhL supplies calibration workflows and recentring calculations
- Detector parameters must be correct
- Shadow compensation calculations require description of precise goniostat shape and mounting angle on the Omega axis
- Beamline file naming conventions (e.g. length of image number mask) must be described to the workflow

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Final words

- We shall be happy to work with you to get the workflow up and running
- The workflow release ships with detailed documentation
- *Automated workflows for strategy computation and data collection at synchrotron beamlines*", Fogh et al. (2026), Acta Cryst D**82** https://doi.org/10.1107/S2059798326001920.
  - Detailed description of workflow program, how strategies are generated and executed, and dose and transmission handling
- "*Radiation damage in sub-Ångström resolution macromolecular crystallography: a low-dose study*", Bourenkov et al. (2026)), Acta Cryst D**82**, https://doi.org/10.1107/S205979832600269X
  - Radiation damage observed at 0.54Å resolution between two datasets, each collected with a 50kGy dose, separated by a 1MGy irradiation.