

Abstract beamline interface for advanced protocols

Global Phasing Ltd.
Peter Keller

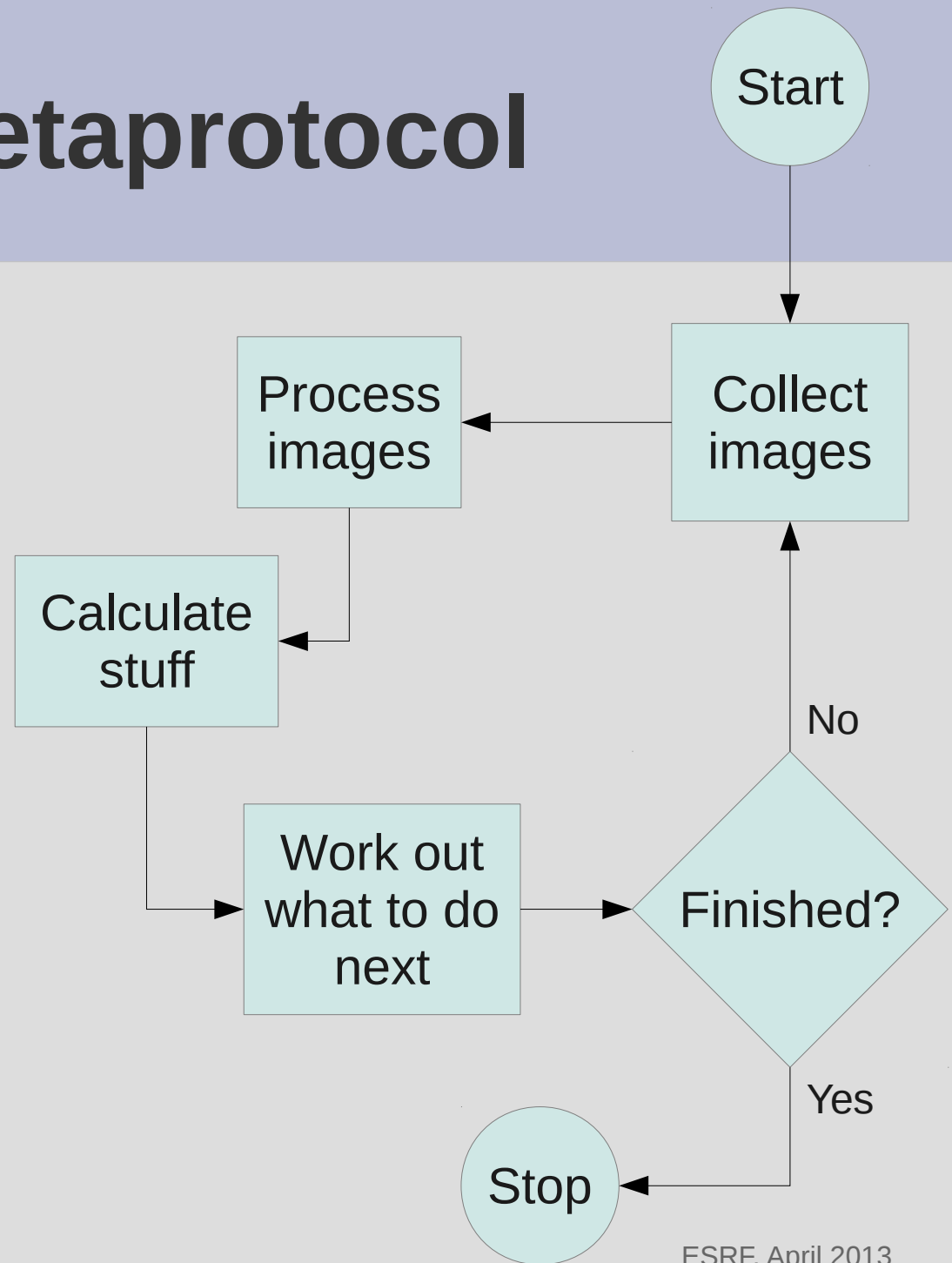
Terminology

- Protocol: Type of experiment required to solve problem
 - Experimental phasing, MR, refinement of a known structure
 - Scientific criteria: completeness, redundancy, ...
 - Testing/calibration of instrumentation
- Strategy: what images to collect next
 - Determined in view of what is known at that point
- Workflow: implementation of a protocol

MX Metaprotocol

The classical MX experiment goes twice around the loop:

- Reference images
- Main data collection(s)



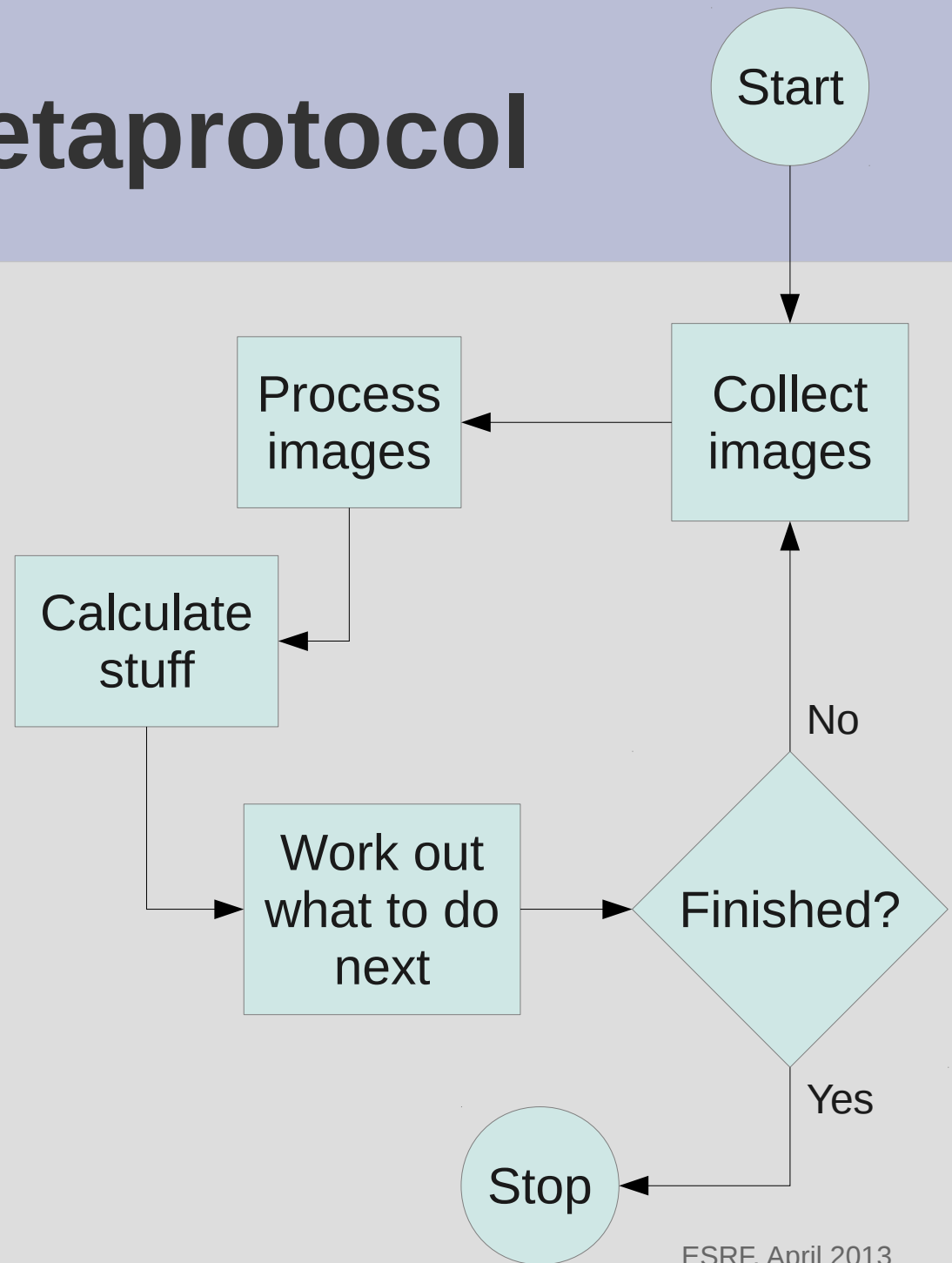
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Global Phasing is seeking to develop new methods and protocols that exploit the capabilities of modern instrumentation to:

- Do successful experiments on intractable samples
- Improve the quality of routine data collection



MX Metaprotocol

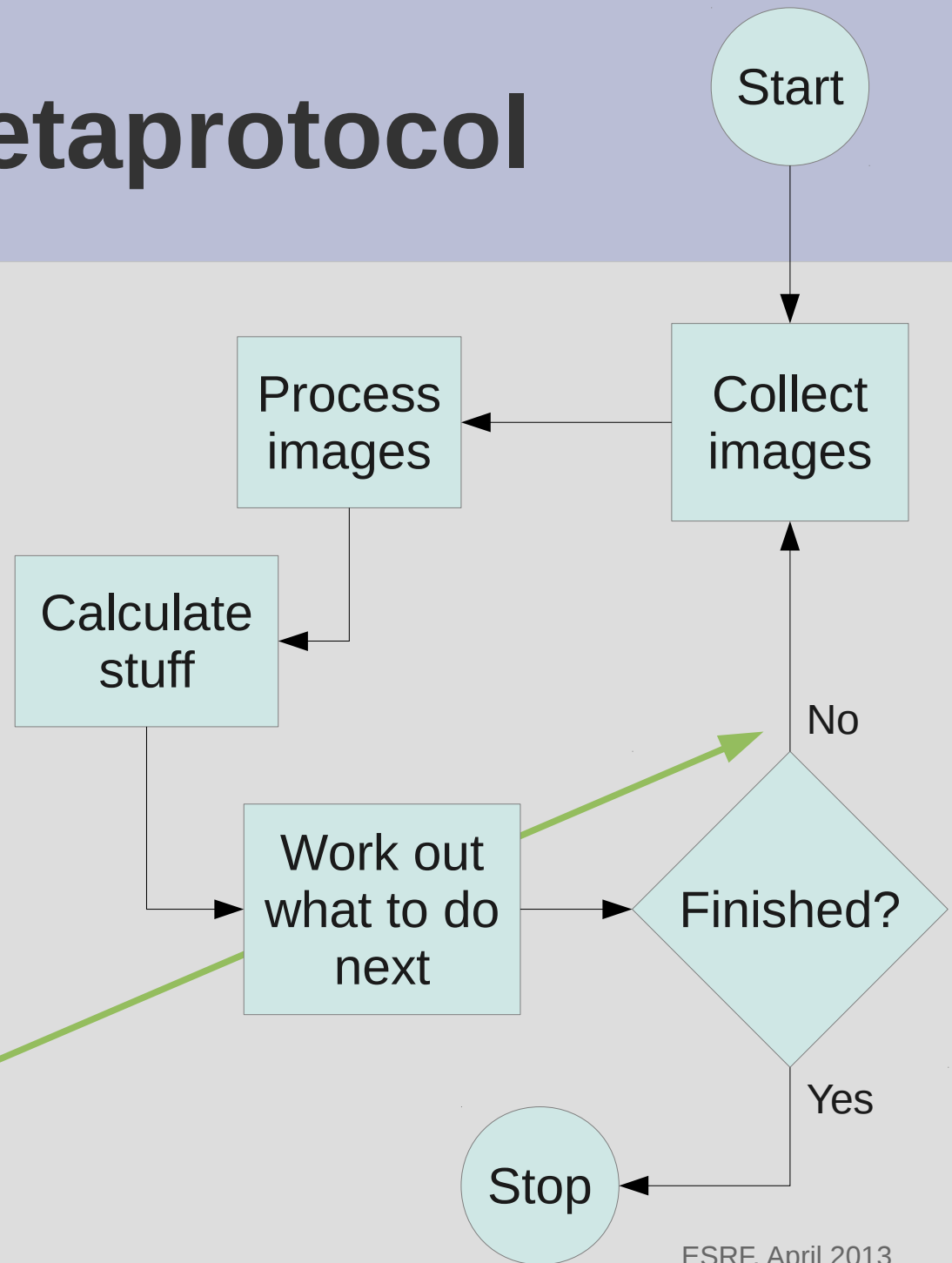
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Transferable automation needed, especially here:



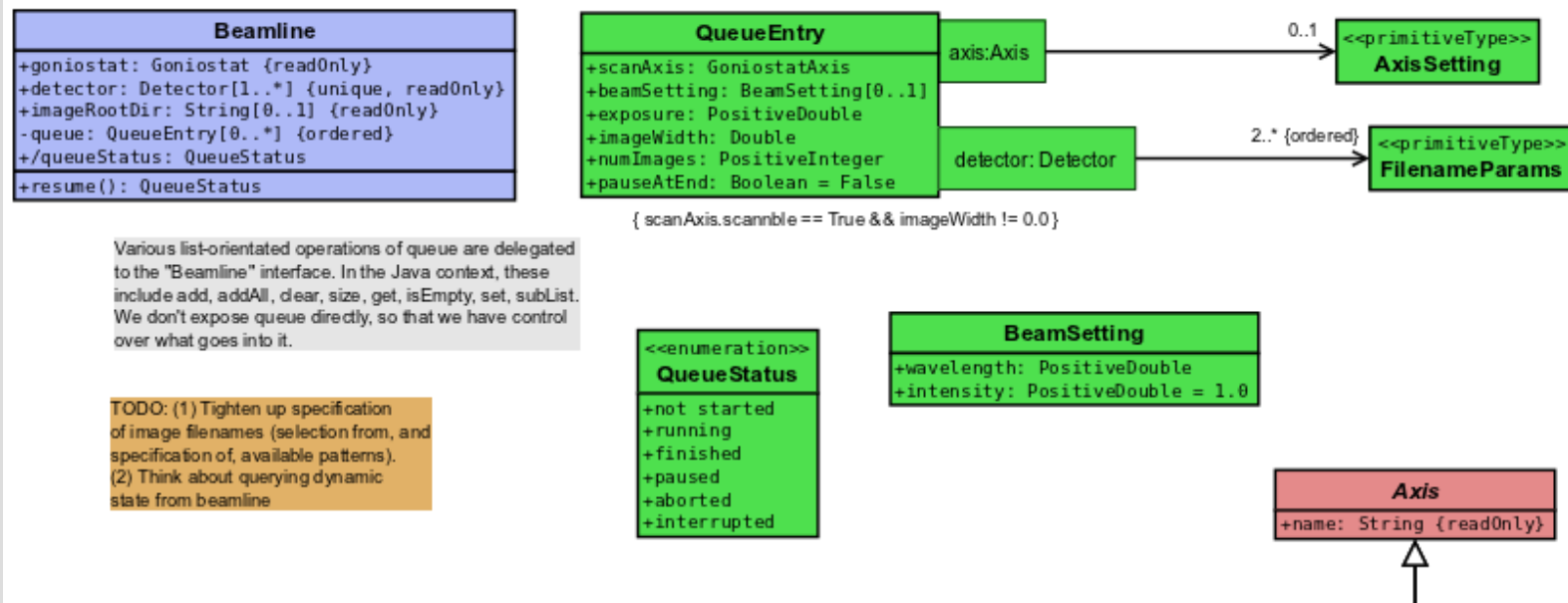
The abstract beamline interface

- Bridge between the reduced and instrumentation views
- Hides settings that are not treated by the reduced view
 - Use “handles” to maintain state of these settings
- Encapsulates beamline-specific procedures
- May have minimal protocol awareness as needed to support local operation modes
 - e.g. known requirements for wavelength switching
- Interface itself needs to be synchrotron-independent

First draft of abstract beamline interface on mxCuBE forum

operational definition of the interface to a beamline that our software will expect to interact with. The Java implementation of it that I am working on at the moment is a hand-written one, not one that is generated by any UML-to-whatever machinery. I hope and expect that the contents of the diagram will remain simple enough so that maintaining implementations by hand will stay tractable.

This interface is a low-level one: it simply performs a sequence of operations. It doesn't "know" that those operations may be the implementation of a particular strategy such as a wavelength interleaved one. Dealing with strategies at a higher level is important of course, but this interface is not intended to do that. Rather, it provides a generic "platform" for a strategy-aware layer to request the collection of images.



Revision needed!

Characteristics of abstract beamline

- Goniostat
 - Only rotation axes represented explicitly
 - Sample assumed to be centred
 - Some interaction with UI has to be catered for
- Detector
 - Geometry: distance, 2θ ; pixel size/number
- Beam
 - Energy/ λ , intensity.

Next steps

- Class diagram defines beamline services that allow a series of sweeps to be collected by software
 - Hides some beamline detail
- GΦL proposes:
 - To develop now a simple experiment driver that uses XML-RPC as the communication protocol
 - MxCUBE developers at participating synchrotrons write a back-end that connects to a real beamline
 - Joint testing and further improvement of the design

Implementations

- Specific to beamline control software
- Technology can vary:
 - GΦL simulator (internal): Java interfaces + implementing classes
 - GDA(DLS/I23): JMS/ActiveMQ message vocabulary has been proposed
 - MxCuBE: XML-RPC with polling (?)
- More tightly coupled to beamline control software than anything else that GΦL currently produces.

Benefits

- Allow externally-generated protocols at participating synchrotrons
- May also be useful for local testing at synchrotrons

Dissemination

- Initial targets
 - MxCuBE
 - GDA
- Other European systems
 - DA+
 - PRIGo well suited to advanced protocols
 - Active collaboration with SLS/PXIII. Some exploratory experiments using interleaving scripts developed jointly with SLS have already been done.
 - More details tomorrow?
 - TAURUS
- Outside Europe