

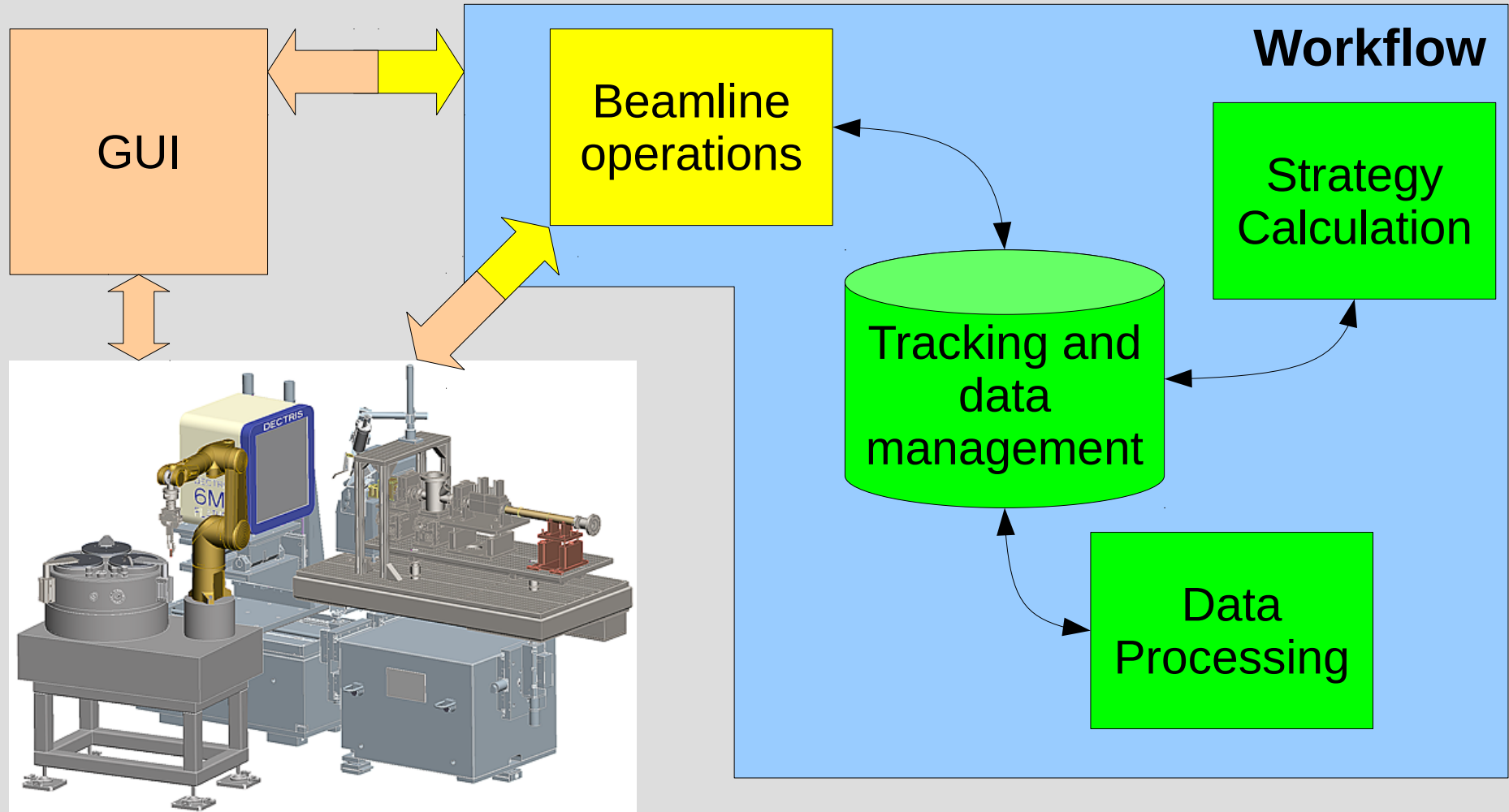
# Presenting GΦL workflow metadata in ISPyB

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# Introduction

- Global Phasing workflows gather a lot of information about the experiment during their execution.
  - Not just what was done, but user choices and strategy calculation, etc.
- In the future, this information could be made available to ISPyB, in whole or in part.

# Transferable workflows



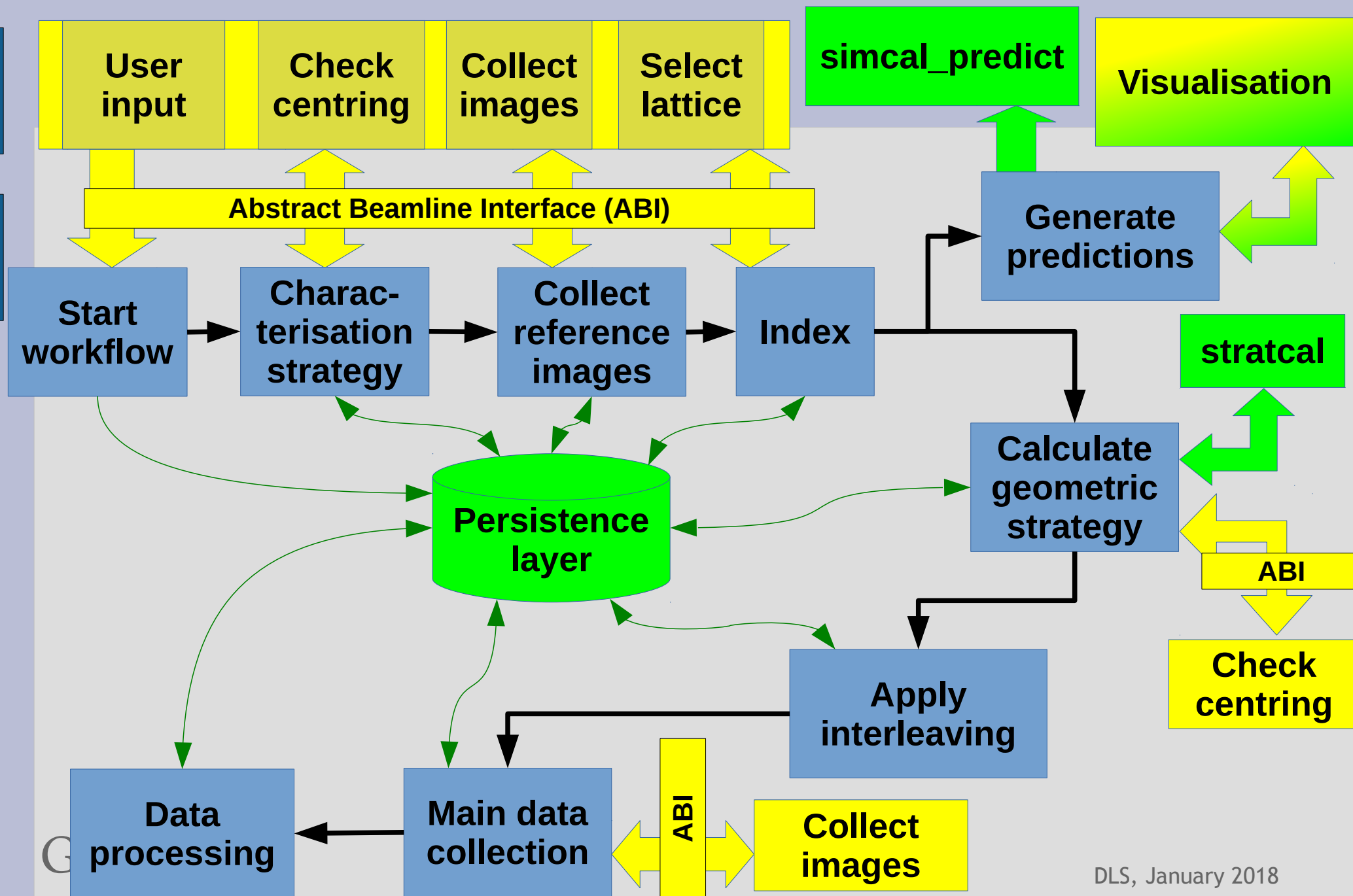
# Abstract Beamline Interface (ABI)

- Defines a vocabulary for communication with a beamline at a scientific level of abstraction
  - Data processing, strategy calculation
- Search for “abstract beamline interface” on GitHub
  - Introduction
  - More explanation (click “Wiki” link on GitHub)
  - UML diagrams
  - Java interfaces

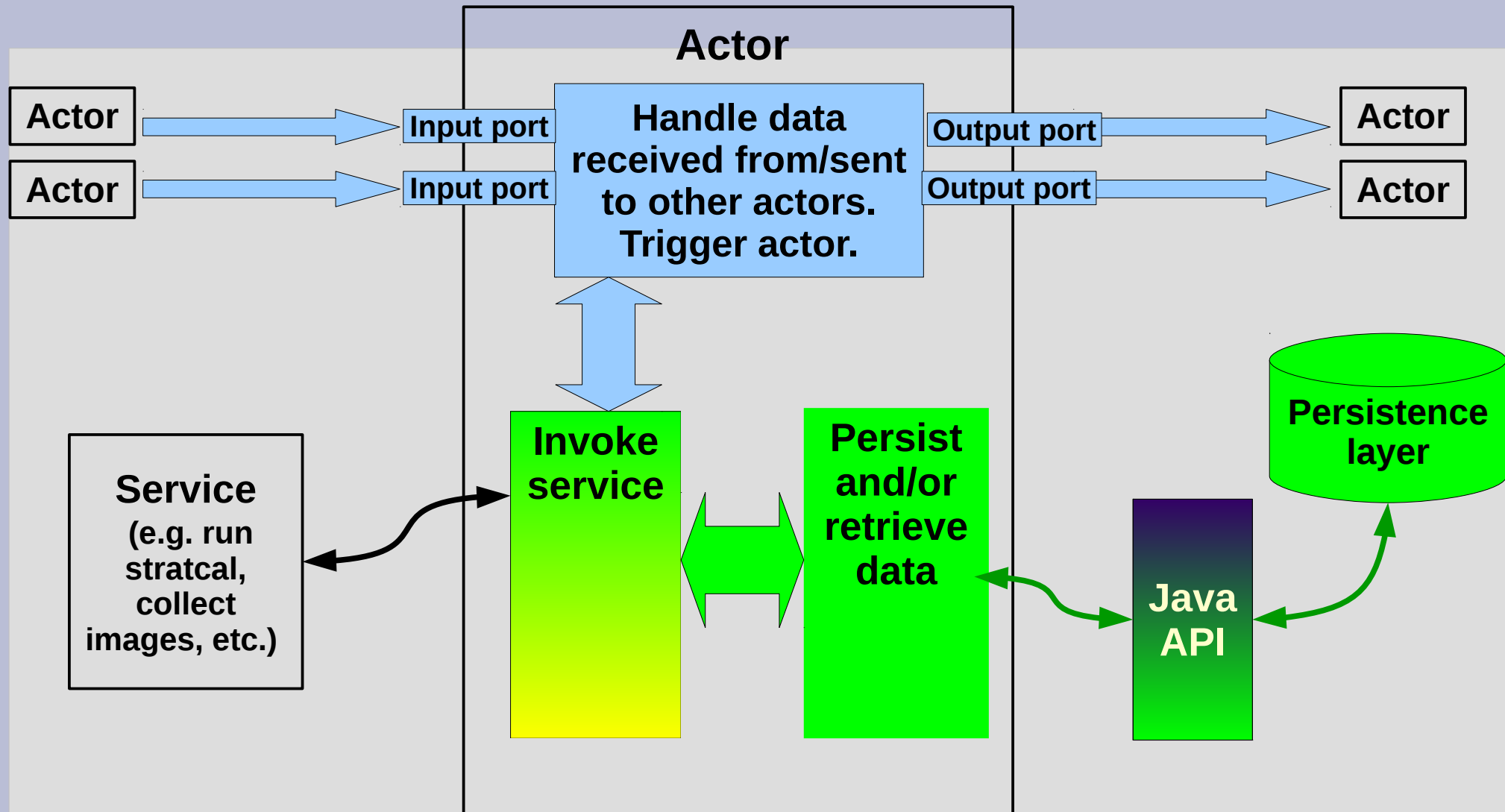
# ABI implementations

- Java Messaging Service (DLS/MXGDA)
  - ActiveMQ message broker
- Py4J (MXCuBE)
  - Direct connection between Rasmus' MXCuBE workflow hardware object and the workflow itself
  - Better suited than the built-in XML-RPC server to this particular task

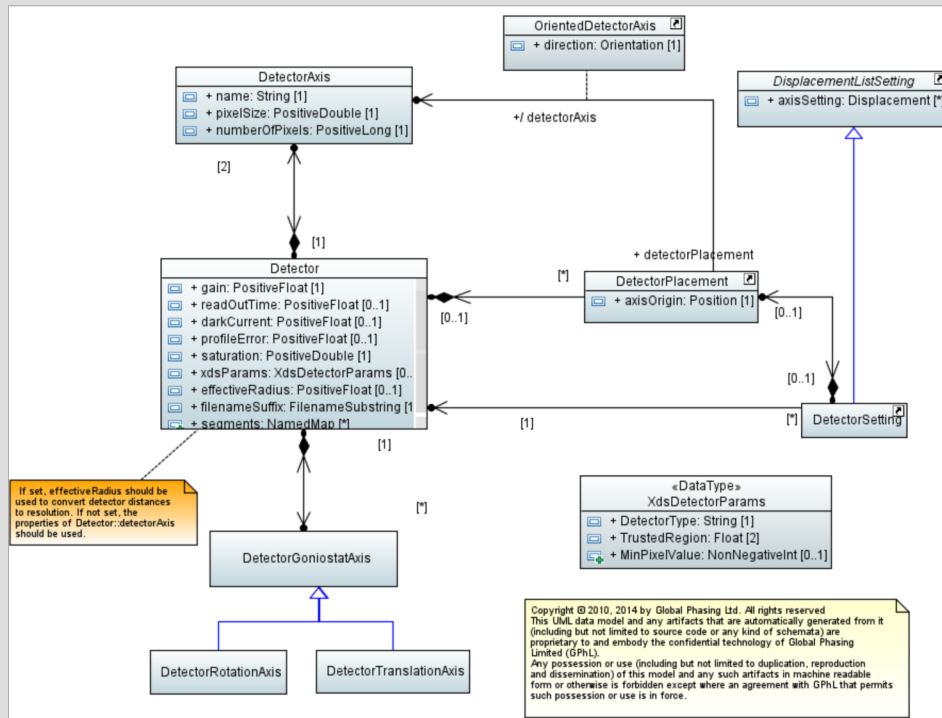
# MX Experimental Workflow



# Anatomy of an actor



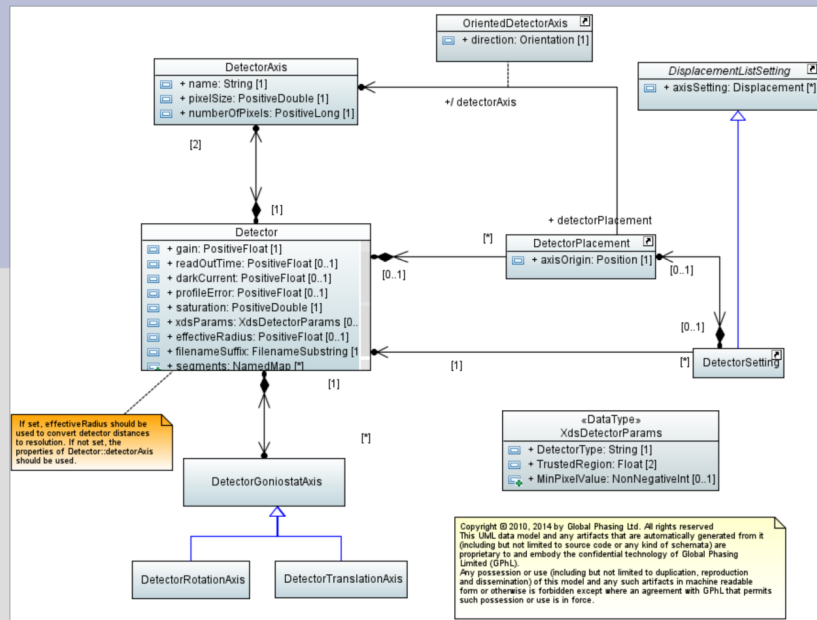
# Persistence layer data model



- About 120 Classifiers
  - Classes,
  - Enumerations,
  - DataTypes,
  - PrimitiveTypes
- About 50 Associations

- Not the same as the Abstract Beamline Interface model





**M2T/EMFT  
(UML to XSD)**

**XML Schemata**

**Manually  
written  
code**

**XMLBeans  
(Generate  
Java  
bindings)**

**M2T/  
EMFT**

**Add API extensions**

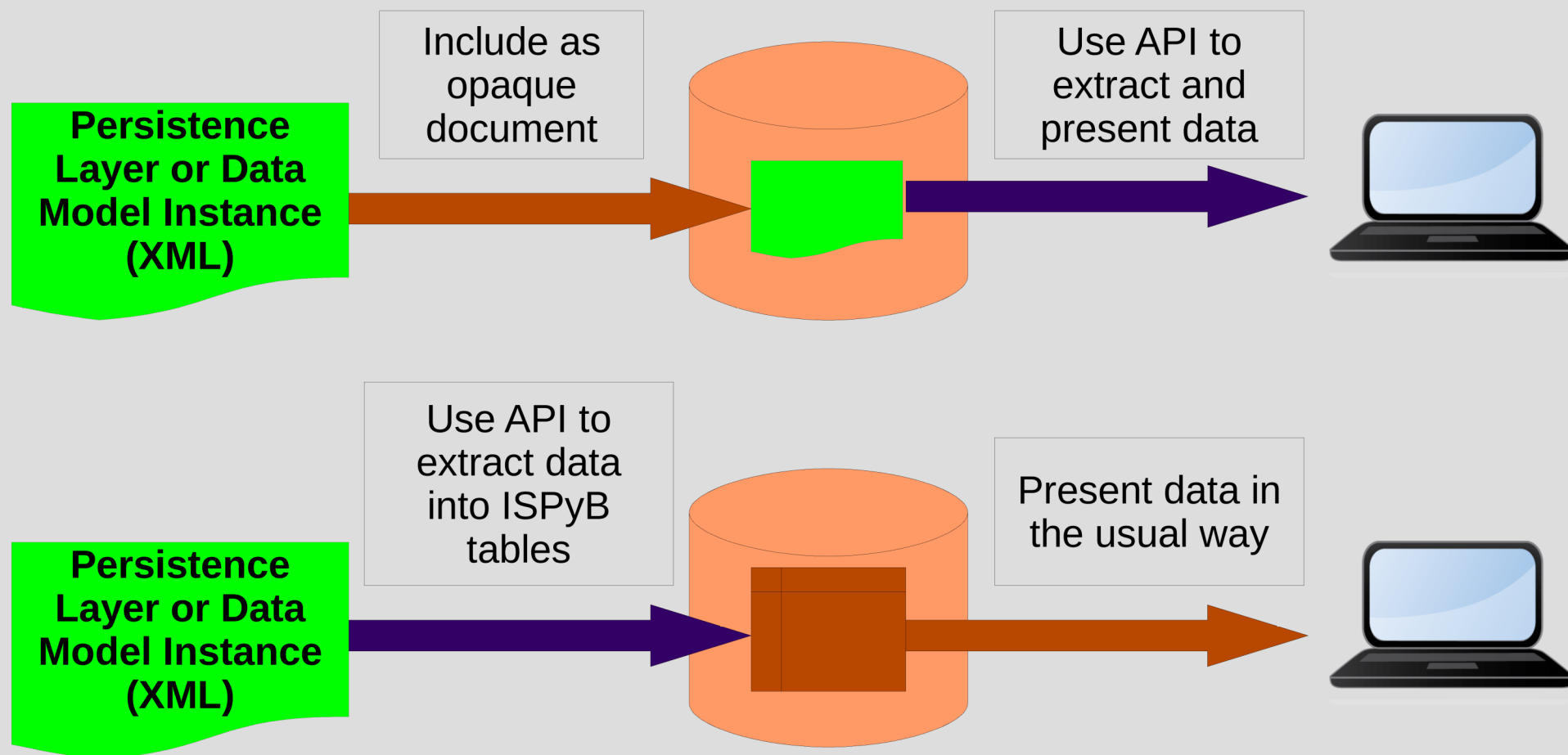
**Extended Java  
API**

**Basic  
validating  
Java API**

**Persistence  
Layer or Data  
Model Instance  
(XML)**

**Model To Text/Eclipse Modeling  
Framework Tools:  
Xpand/Xtend and Modeling  
Workflow Engine**

# Future link-up with ISPyB?



# Versioning

- Data model versions identified by date
  - Model change  $\Rightarrow$  XML schemata & API change
  - Particularly important for “on-the-fly” extraction
- Application must use matching API version
  - Accessing a data model instance with the wrong version of the API produces a validation error
- XML Schema namespaces are 'tag' URIs
  - RFC 4151: the syntax requires a date
  - Namespaces look like:  
`tag:globalphasing.com,2017-09-27:schemata:SDCP/Core`

# Acknowledgements

- GΦL: Gérard Bricogne, Claus Flensburg, Rasmus Fogh, Wlodek Paciorek, Clemens Vonnrhein
- DLS: Jon Blakes, Ramona Duman, Kamel El Omari, Richard Fearn, Ralf Flaig, Dave Hall, Paul Hathaway, Vitaliy Mykhaylyk, Pierpaolo Romano, Armin Wagner, Graeme Winter
- ESRF: Antonia Beteva, Matias Guijarro, Marcus Oscarsson
- EMBL-Grenoble: Andrew McCarthy