ISPyB for XPDF

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ESRF ISPyB Meeting
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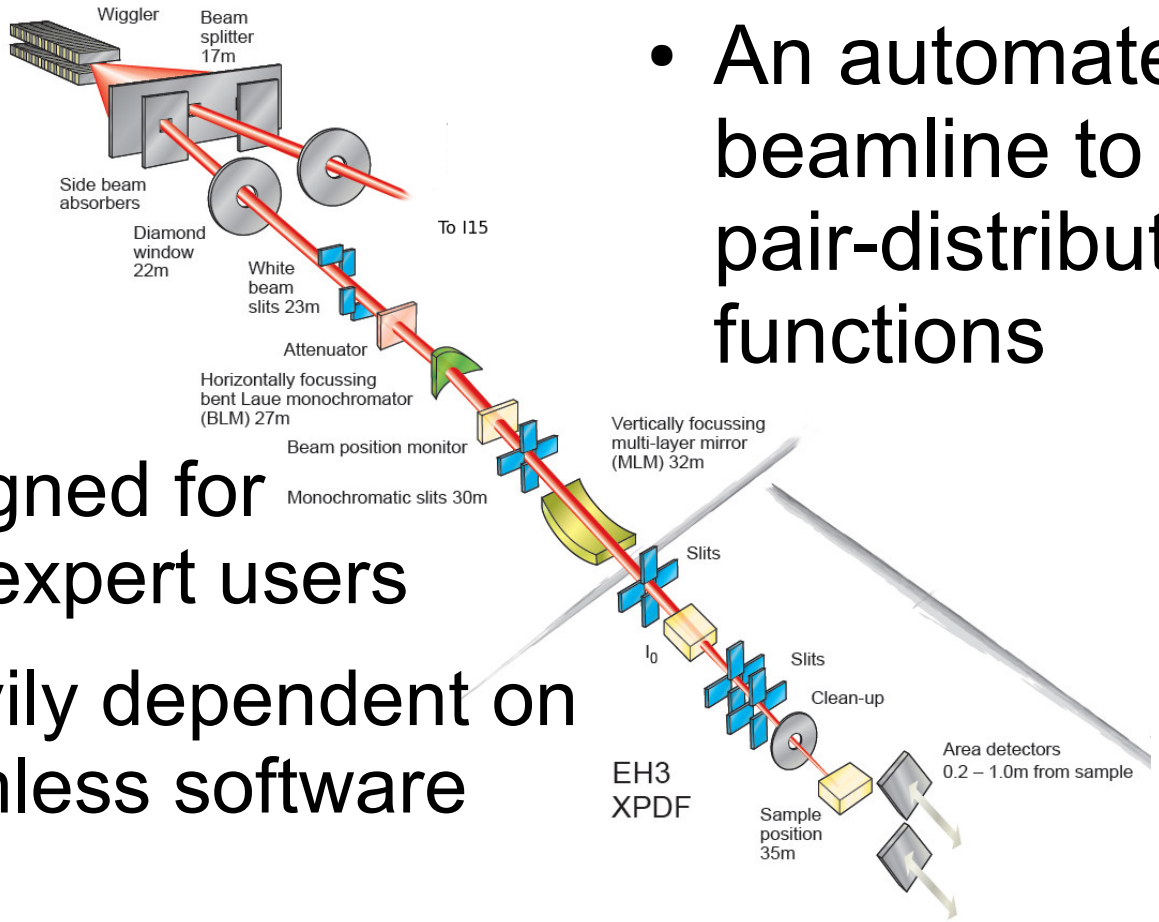
The XPDF Project



- An automated beamline to produce pair-distribution functions
- Designed for non-expert users
- Heavily dependent on seamless software

XPDF Requirements

- Upload sample composition data
- Create plans for the experiment
- Process the beamline data automatically
- Allow access from user's institutions

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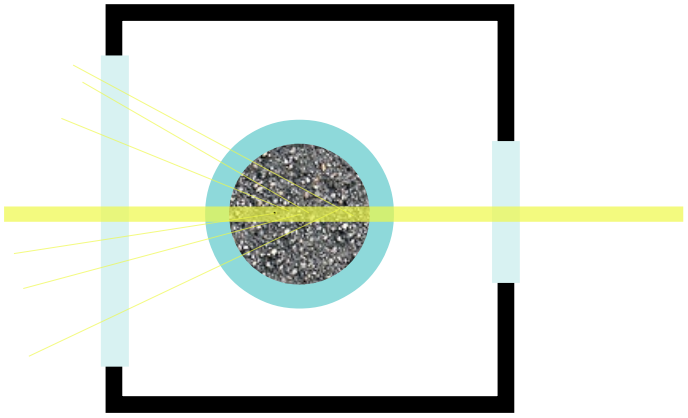
Why use ISPyB?

- Already exists
- Expertise in-house
- Deals with the difficult parts of LIMS
  - Remote access
  - Data security
  - User interface

Samples and Phases

- A user's sample is a mixture of several powder or amorphous phases
- Each sample can be packed into several containers
- Data collection is performed on each ‘instance’



Mapping from MX to XPDF

- ISPyB BLSamples have data collected on them, XPDF samples do not
- ISPyB containers are used for shipping and sample grouping, XPDF containers physically hold the sample to be imaged
- XPDF processing needs parameters that MX does not

Proteins → Phases

- Each has a composition
- May be found in many samples
- Each sample may have many phases
- A phase has a crystallographic density
- In a powder, each phase can have a different lattice

Crystal → Sample

- Crystal loses its importance with respect to lattice parameters and physical dimensions
  - Lattice parameters → Phase
  - Physical size → Instance
- An XPDF sample is a collection of phases, with abundances

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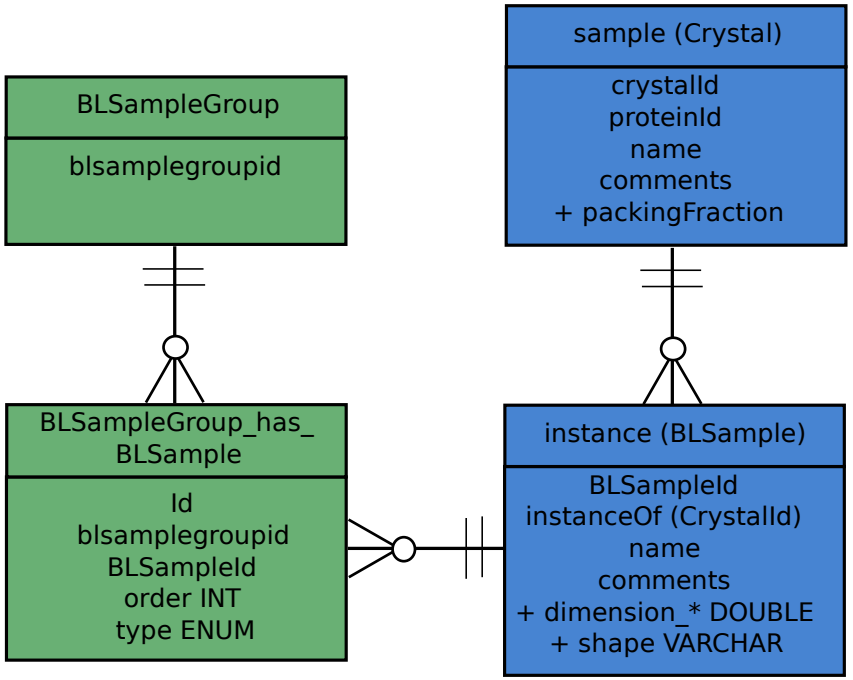
Containers and Instances

- Each instance of a sample is stored as a BLSample
- An instance is distinguished by being contained by a container
  - Physical size
- Containers are also BLSamples, with Crystals and Phases for composition
  - Can be shared between experiments
  - Have data collections associated with them

Containers and Instances

- Extra semantics are needed for the containers
- Need an ordered set of containers to calculate fluorescence, scattering and absorption



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DiffractionPlan *&c.*

- Parameters to be varied during an experiment associated with a DiffractionPlan
- Multiple DiffractionPlans can be run on a sample
- One or two Detectors associated with a DiffractionPlan
- Detector material and areal thickness

Summary

- ISPyB can be adapted for new experiment types
- New columns must be added for parameters important to the type of experiment
- New tables can be needed when the semantic structure of the data to be stored is different