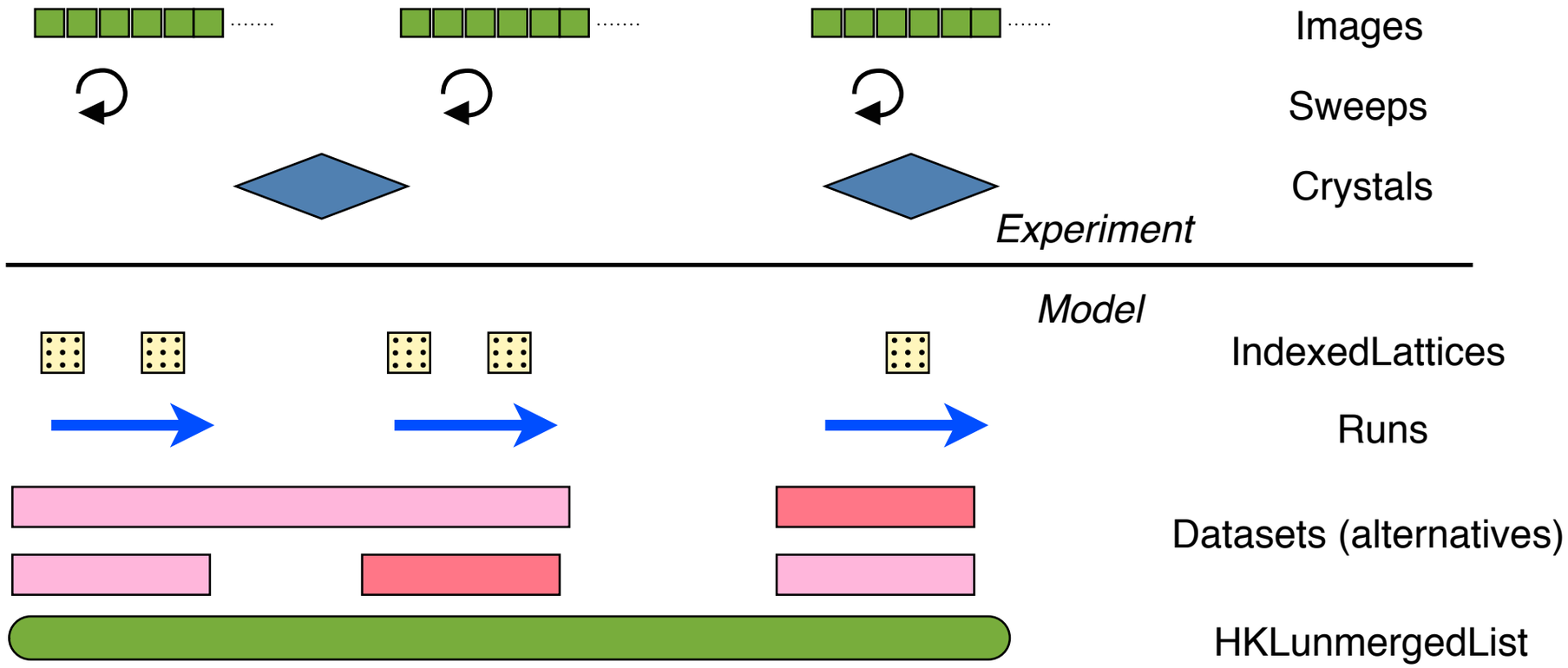
At the Developer's meeting I promised to "design" a data model

... but I haven't done it

My excuses: other things done

- multi-lattice stuff: Feckless, Pointless, Aimless
- TILE correction for 3x3 tiled CCDs
- investigation of SDCORRECTION problems – inconclusive

Data objects for unmerged data: an outline proposal for discussion



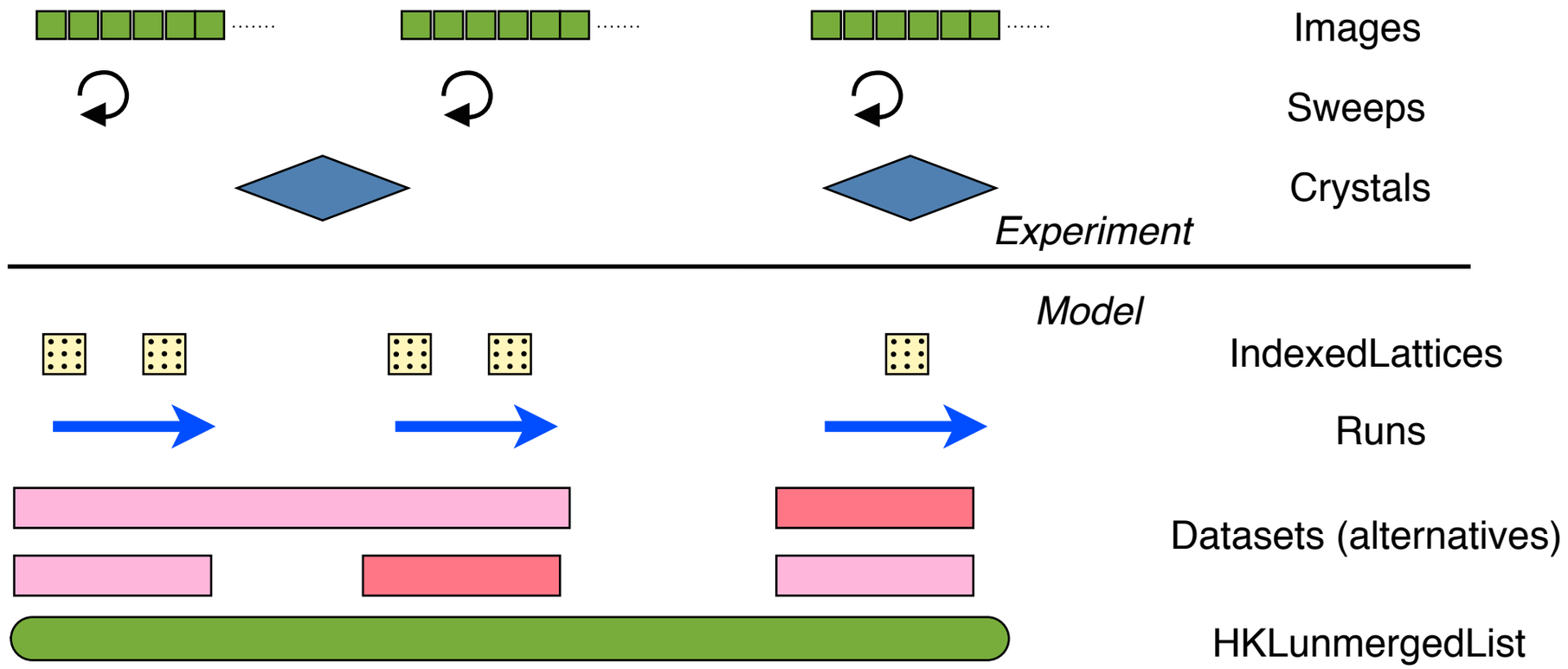
Why?

Current storage both in my internal classes and in MTZ file does not reflect the experiment and its interpretation properly, and is a problem with multiple lattices.

Some aspects of the experiment are not stored explicitly in the MTZ file, notably *Sweep* which is the fundamental unit of data collection

Both my classes and MTZ store a BATCH which mixes up information from:

1. instrument description: goniostat [and should include detector] – belongs to *Sweep*
2. rotation range (φ_{start}, φ_{end}) – belongs to *Sweep*
3. crystal mosaicity – belongs to *Crystal*
4. cell, crystal orientation – belongs to **one** *Lattice*, a problem with multiple lattices



Top 3 classes describe the experiment: put crystal in beam, rotate, collect contiguous images

A *IndexedLattice* is an indexing, with cell, orientation, and (ultimately) space group

Run is just a list of lattices for a sweep

A *Dataset* is what you choose to combine for further processing, eg one wavelength of a MAD set, etc

HKLunmergedList is a container for everything, including the actual reflection/observation/part list (as now)

May also need a *Batch* class to link an observation to its *Lattice* and *Crystal*/*Sweep*/*Image* (essentially a lookup)

Properties of each object class to be determined! (I have an initial outline, based on current usage)

Experimental data:

This looks like dxtbx!

Red indicates a class

- ***Sweep***:
  GoniostatSweep
    GoniostatDefinition
    angular range, sweep axis
    Rotation range/Image
    exposure time/Image
  Beam
    direction, wavelength, dispersion, divergence, polarisation, size, [intensity]
  Detector
    all the detector parameters
  Reference to ***Crystal***
  [list of images (?implicit)]
  [elapsed time/date]
  Beamline
  Reference to ***Run***s
- ***Crystal***:
  Crystal Name
  [full geometry description]
  list of [references to] ***Sweep***s

IndexedLattice

Cell unit cell etc → [**B**]

[estimated errors in unit cell]

Symmetry (space/Laue group)

symmetry status

cell constraints

CrystalOrientation

[**U**]

Mosaicity

? anisotropic

mosaic block size

reference to ***Run***

reference to ***Sweep***

Run (for one ***IndexedLattice***)

run number

reference to ***Sweep***

reference to ***IndexedLattice***

Dataset

name

list of ***Run***s to use for dataset

Batch (used to get from observation list to other information)

reference to ***Run***