1 Introduction

The application `xia2scan` is designed to scan through a list of provided images and print information about the "quality" of the diffraction on the images. This will end up as an executable `xia2-scan(=> .sh/.bat)` and a python program xia2scan.py.

1.1 Appication

This is designed to be useful for

- Selecting the best images for autoindexing from a sweep.
- Optimizing humidity when a humidifier is available.

by printing information about the strength of diffraction in each image.

2 Uses...

This uses the wrappers for labelit.screen and labelit.stats_distl.

3 Dependencies

This application will depend on having access to a user provided beam centre (by implication then an input argument / command line handler) and also diffraction image name parsing to allow searching of a directory for matching images.

4 Use Cases

4.1 UC 1: Humidifier

Requires:

- The correct beam position (for indexing from single images.)
- The images.

Provides:

- The statistics for each image in the list.

4.2 UC 2: Indexing Image Selection

This will scan through all of the images in a sweep and select, based on the spot separation and so on, the best pair for autoindexing.

5 Implementation

5.1 UC 1: Humidifier

This will use the following classes:

- Schema.Sweep.SweepFactory - to generate a list of sweeps from the images provided.
- Handlers.CommandLine - to hold the beam centre information from a previous indexing run.

To achieve reasonable speed, the labelit run will not optimise the beam centre (this is unreliable from a single image anyway) and also will run the labelit before distl, and use labelit.stats_distl to get the results afterwards.

This should do all of the running, then collate the results and print a summary. The following arc should be followed:

- [determine accurate beam centre]
- Digest matching frames to list of sweeps.
- For each sweep, run labelit, get an idea of the unit cell volume, run labelit.stats_distl to get the intensity summary, save.
- Print summary by image number.

5.1.1 Test Data

Rajan provided me with a couple of test data sets - use these. Oh bugger - the images are stills... Add a special case in the sweep factory to return these as separate frames? Or just plough ahead??