Project X: New Approach to Still Shot Processing

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1 Problem

At the moment accurate refinement of still shot data presents problems where central impacts are used, as the assumption that the full reflection has contributed to the centre of mass of the observed spot is manifestly false. Methods to address this typically rely on estimating some correction factor based on the crystal mosaicity, but these are inherently dependent on the choice of mosaicity model and also are not able to take the *absence* of a reflection into consideration.

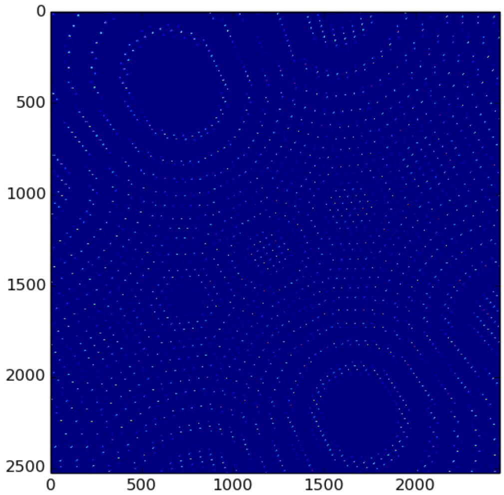
2 Suggestion

Given an indexed diffraction pattern, a Miller index may be computed for any position on the detector, be this a reflection or no. Of course, most of these indices will be non-integral, and the index assigned is entirely dependent on the current orientation matrix and unit cell. The option however exists to compute an "image" of the distance to the nearest integral reciprocal lattice point (relp) or some function of this distance for every pixel, and compare this with the observed pixel data. If a function is used which rapidly decreases as the distance from the relp increases, the resulting map should look similar to the original diffraction image if the length scale for the fall off is comparable to the reciprocal space size of the observed reflections.

This therefore gives the opportunity to compute a penalty function not as the observed gap between observed and predicted spots, but instead to use the similarity of the observed pixel data to the calculated distance function: if relps are close to reflecting position they should be observed, and if they are not observed this may be used to guide model improvement.

Proposed penalty function: correlation of calculated distance function with observed pixel data - maximising this should result in a good model of the data.

For example image 9 (one lattice) this gives an image like:



This was calculated with a 3D Gaussian with $r = 0.1$ i.e. corresponding to a sphere around each relp - here there are clearly more spots than were measured, so in this case r is too large. Also spots were only observed to around 1.8Å, so some kind of B-factor model will be needed.

3 Issues

This is computationally expensive to evaluate, particularly with the current Python code. Probably impossible to get analytical derivitives. To make function vary smoothly as the model parameters are changed may require integration of the distance function across each pixel rather than taking the central value, particularly if the pixels are large when compared with the spot.

Actually integrating the data following this could use the computed distance function as a proxy for the reflection profile, and this would give an opportunity to derive a useful scale factor at the same time.