An implementation of XDS integration for DIALS

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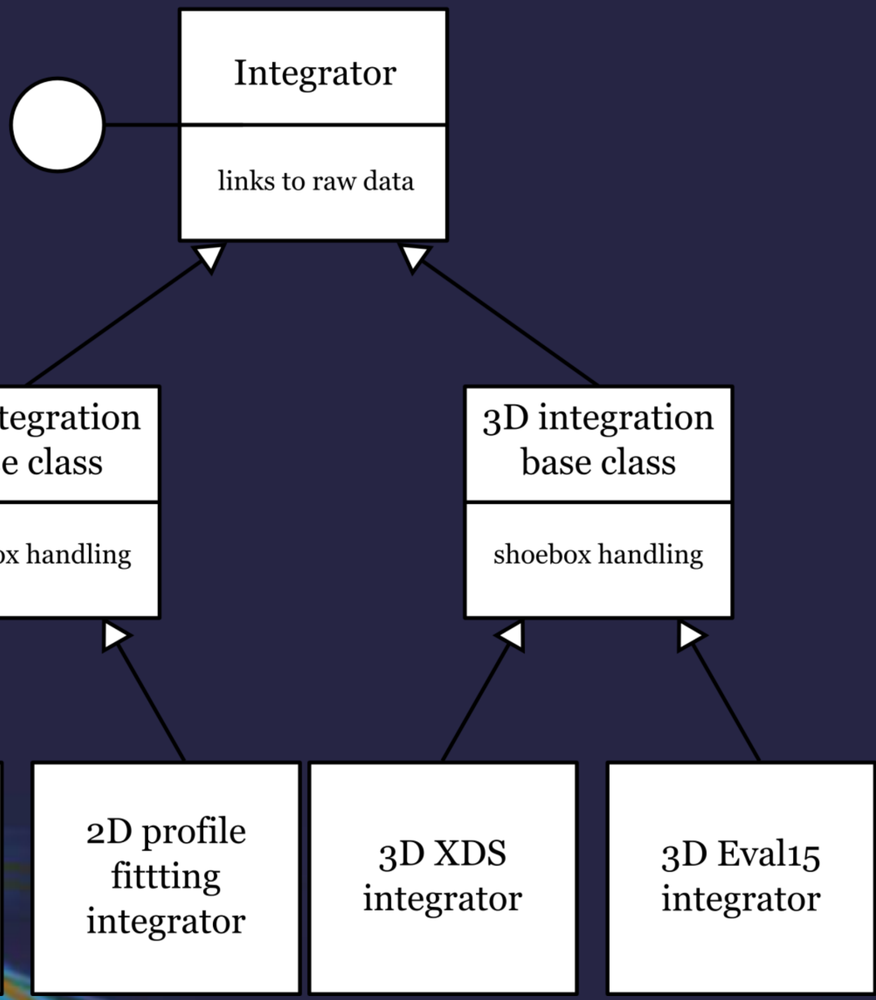
Design principles (interfaces)

Integrator hierarchy

See Graeme Winter's talk



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XDS

- Program for processing single-crystal monochromatic diffraction data recorded by the rotation method

- Differs from other 2D integration programs such as Mosflm by integrating reflection profiles in 3D

- Described in Kabsch, W. (2010). Integration, scaling, space-group assignment and post-refinement. *Acta Crystallographica Section D Biological Crystallography*, *66*(Pt 2), 133–44.

Overview

- Modeling rotation images
  - Spot prediction
  - Localizing diffraction spots
  - Basis extraction
  - Indexing
  - Refinement
- Integration
  - Reflection mask
  - Background subtraction
  - Reciprocal space transform
  - Intensity Estimation

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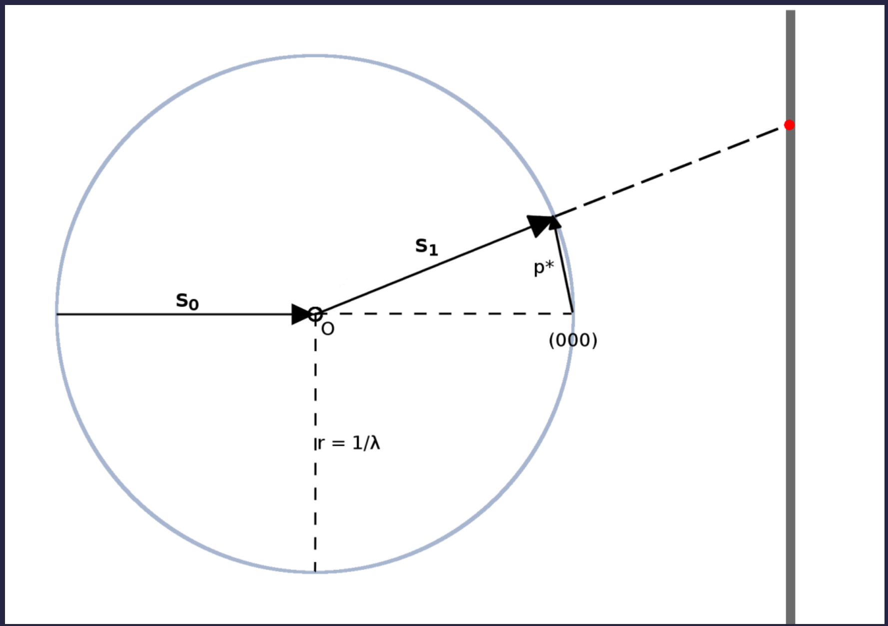
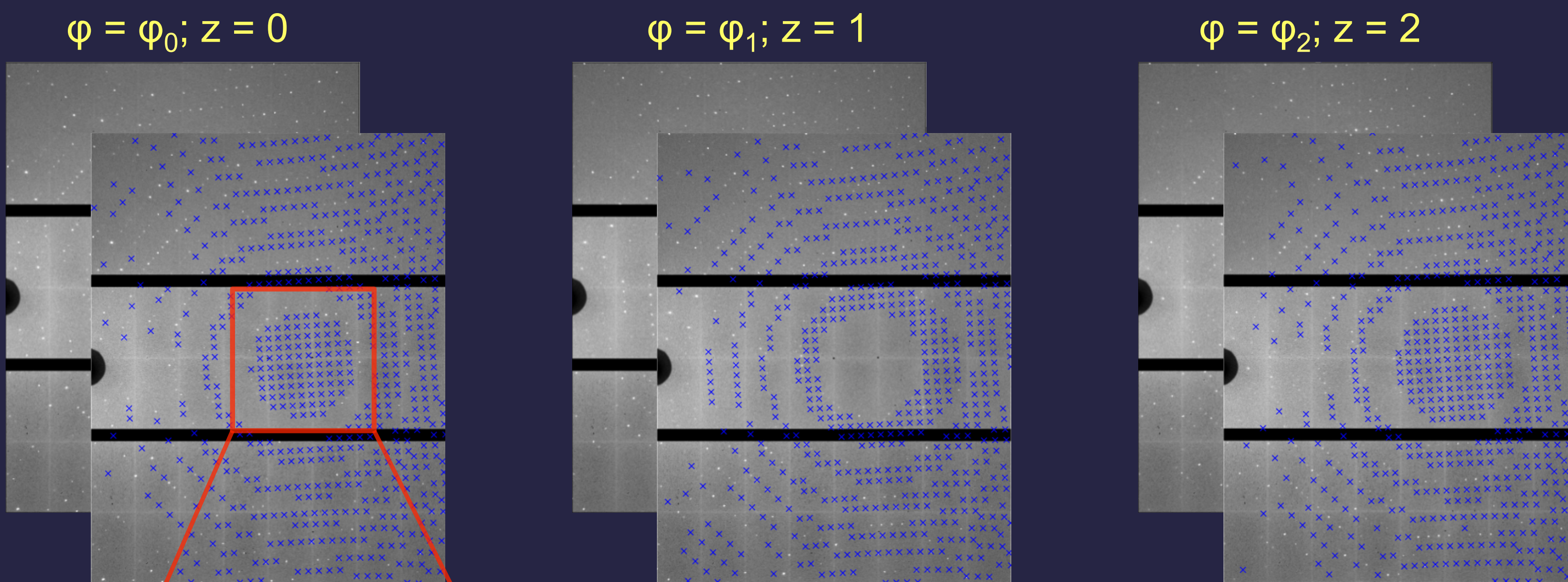
Spot prediction: method

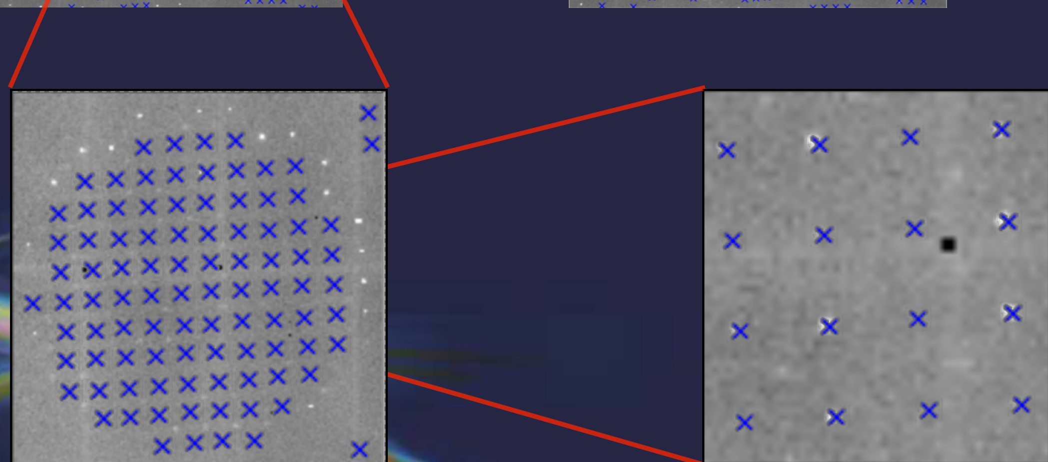
- Purpose: To obtain detector coordinates and rotation angles for each predicted reflection

- Generate observable miller indices
- For each index calculate:
  - intersection angle with Ewald sphere
  - diffracted beam vector
  - intersection point of diffracted beam vector with detector plane



Spot prediction: results





Spot positions validated to within 0.1 pixels w.r.t refined XDS spot positions

Reciprocal space transform: coordinate system

Definition:

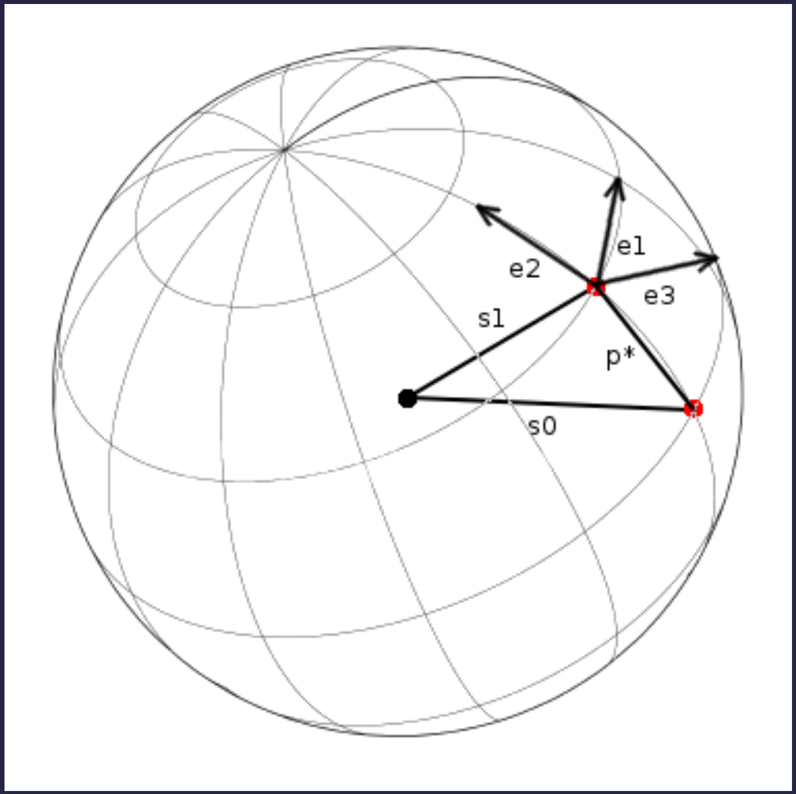
$$\boldsymbol{e}_1 = \boldsymbol{S}_1 \times \boldsymbol{S}_0 / \, |\boldsymbol{S}_1 \times \boldsymbol{S}_0|$$

$$\boldsymbol{e}_2 = \boldsymbol{S}_1 \times \boldsymbol{e}_1 / \, |\boldsymbol{S}_1 \times \boldsymbol{e}_1|$$

$$\boldsymbol{e}_3 = \boldsymbol{S}_1 + \boldsymbol{S}_0 / \, |\boldsymbol{S}_1 + \boldsymbol{S}_0|$$

Motivation:

- Rotation about a fixed axis leads to an increase in the path length through the Ewald sphere.
- Transformed reflections have a standard shape and appear to have followed the shortest path through the Ewald sphere.



Reciprocal space transform: mapping

Formula

$$\varepsilon_1 = \boldsymbol{e}_1 . \frac{(\boldsymbol{S}' - \boldsymbol{S_1})}{|\boldsymbol{S_1}|} \times \frac{180}{\pi} \qquad \varepsilon_2 = \boldsymbol{e}_2 . \frac{(\boldsymbol{S}' - \boldsymbol{S_1})}{|\boldsymbol{S_1}|} \times \frac{180}{\pi}$$

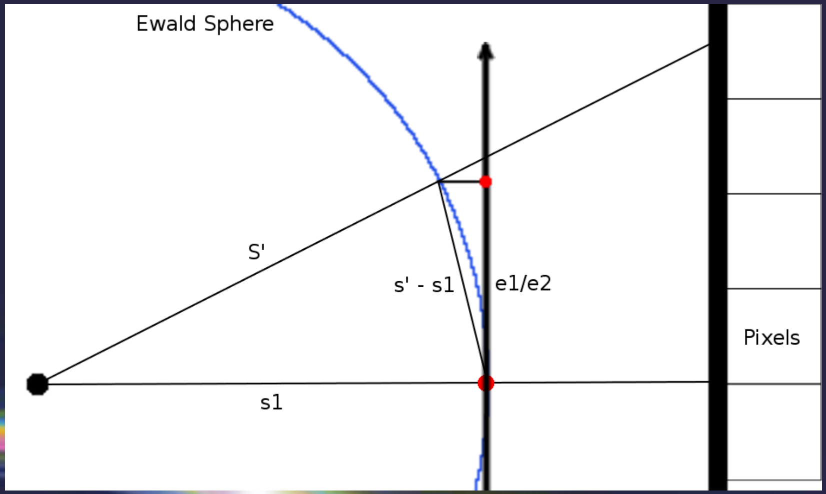
$$\varepsilon_3 = \boldsymbol{e}_3 . \frac{[R(\boldsymbol{m}_2, \varphi' - \varphi)\boldsymbol{p}^* - \boldsymbol{p}^*]}{|\boldsymbol{p}^*|} \times \frac{180}{\pi} \approx \zeta . (\varphi' - \varphi)$$

ζ is related to the inverse Lorentz correction factor.

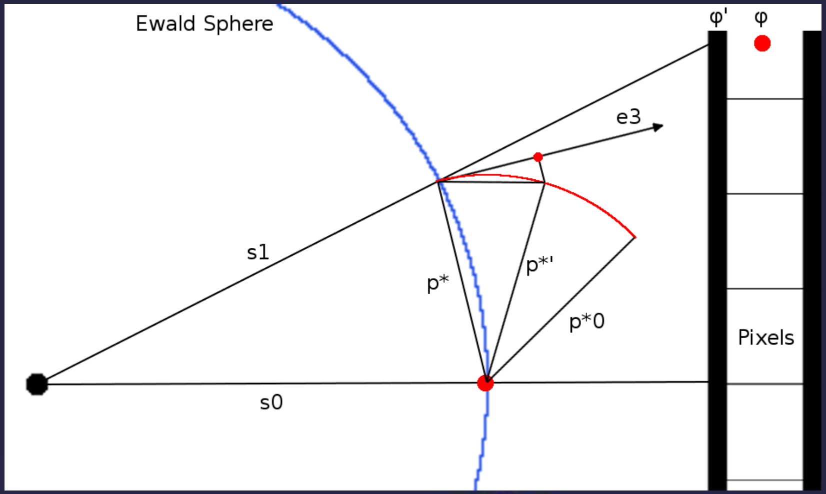
$$\zeta = \boldsymbol{m}_2 . \boldsymbol{e}_1$$

$$L^{-1} = \frac{|\boldsymbol{m}_2 . (\boldsymbol{S_1} \times \boldsymbol{S}_0)|}{|\boldsymbol{S_1}||\boldsymbol{S}_0|} = |\zeta \sin \angle(\boldsymbol{S_1}, \boldsymbol{S}_0)|$$

e_1/e_2 transform



e_3 transform



Reciprocal space transform: required steps

Calculate reflection mask

↓

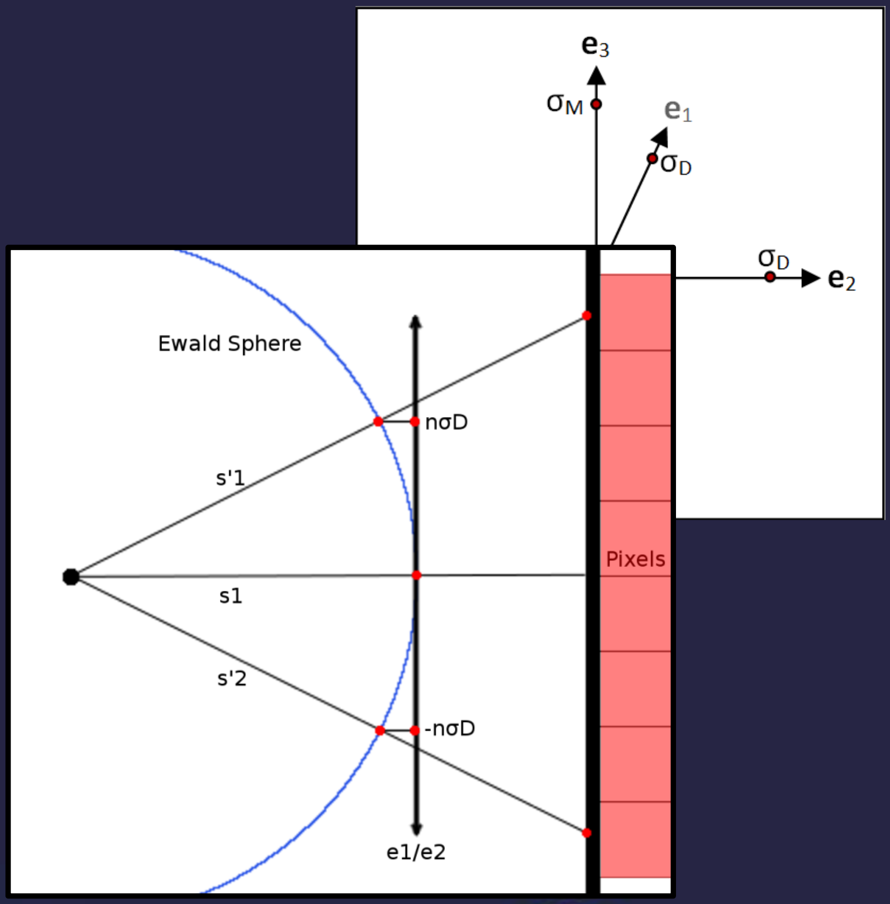
Subtract background intensity

↓

Perform reciprocal space transform

Reflection mask: calculating the shoebox

- Reflection mask uses standard deviation of beam divergence (σ_D) and mosaicity (σ_M) in reciprocal space to set shoebox around each reflection
- shoebox <= $|n\sigma_D|\mathbf{e}_1$, $|n\sigma_D|\mathbf{e}_2$, $|n\sigma_M|\mathbf{e}_3$
- Detector coordinates and rotation angles at limits are calculated to obtain shoebox in detector space
- Results in shoebox specific to each reflection



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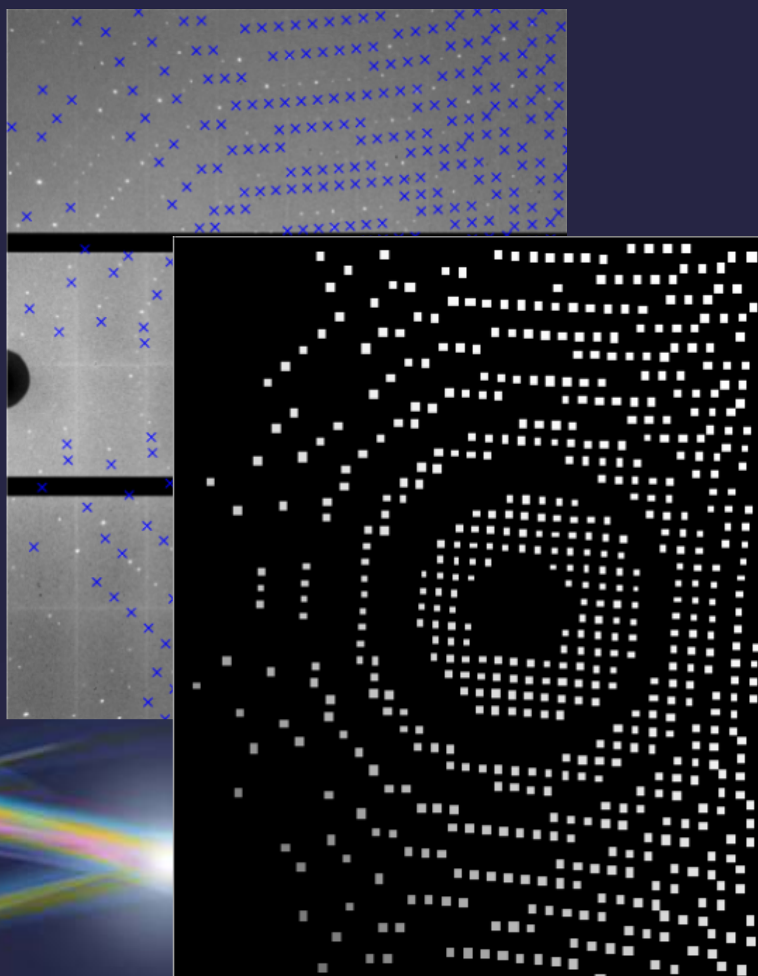
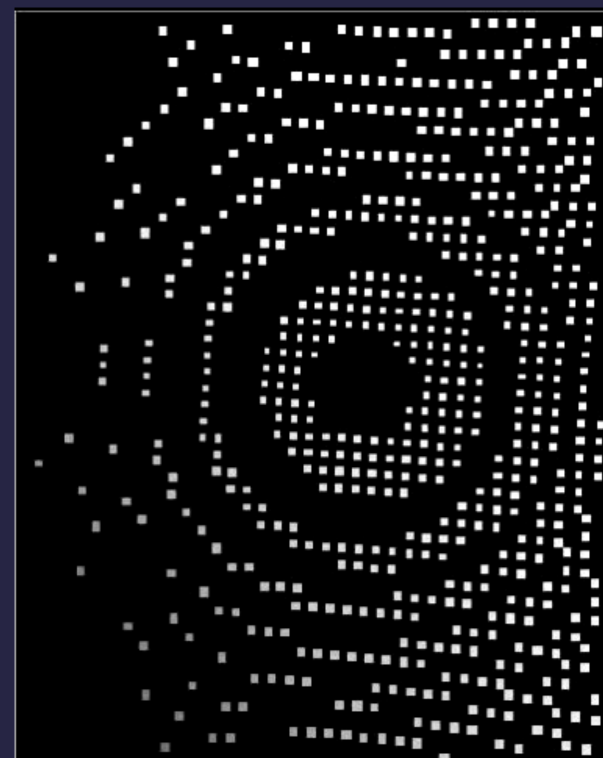
Reflection mask: images

Single frame:



Whole dataset:



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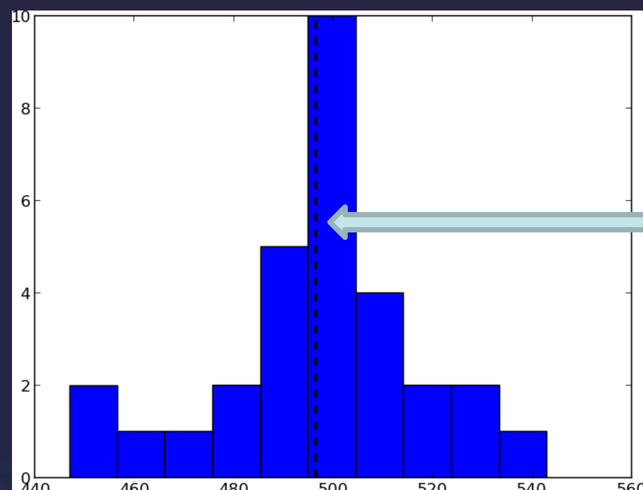
Background subtraction: method

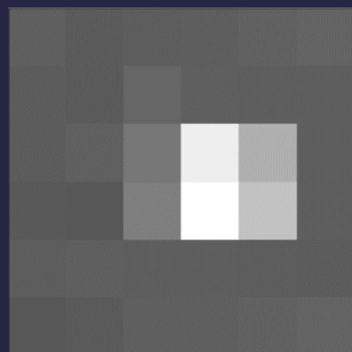
- Assume enough pixels available (> 10) to calculate background
- Assume background intensity distributed normally
- Remove high intensity pixels, one at a time, until intensity is normally distributed
- Select mean of remaining pixels as background intensity

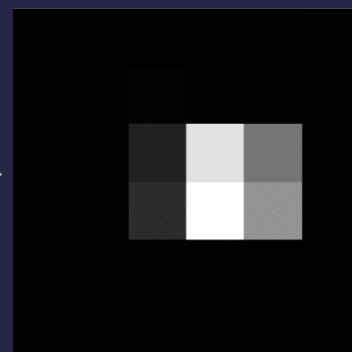


Background intensity value

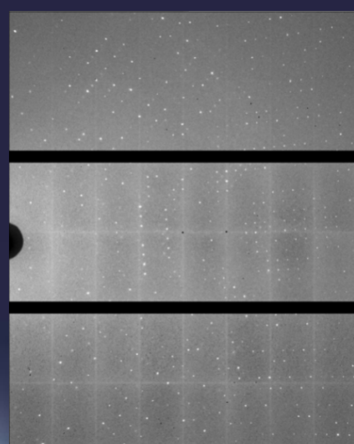
Background subtraction: results

Single spot:





Whole frame:



Whole dataset

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Reciprocal space transform: gridding frames

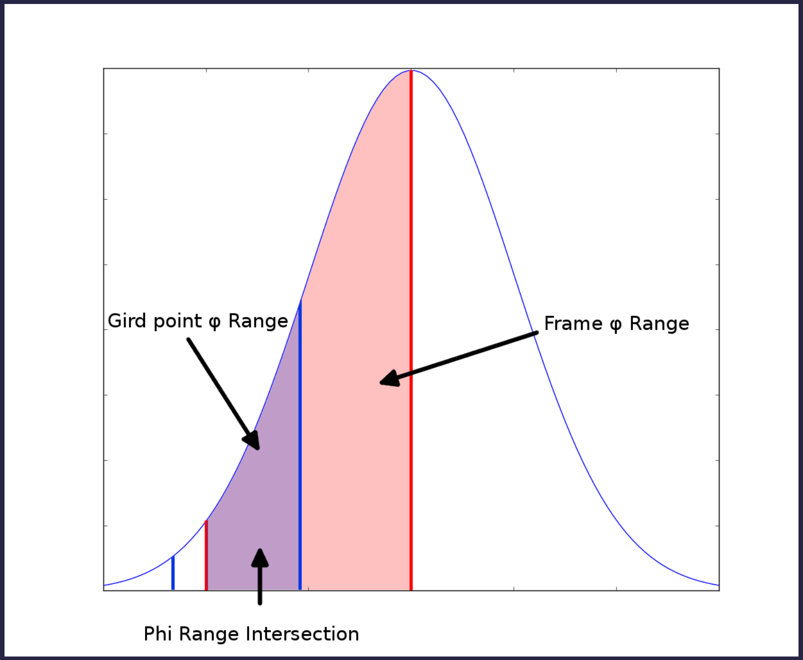
- Assume Gaussian spot profiles along $\mathbf{e}_3$
- Integrate over range of φ for the image frame, j:

$$I_j = \int_{\Gamma_j} \exp(-(\phi' - \phi)^2 / 2\sigma^2) d\phi'$$

- Integrate over the intersection of the range of phi range of the grid point v_3, and image frame, j:

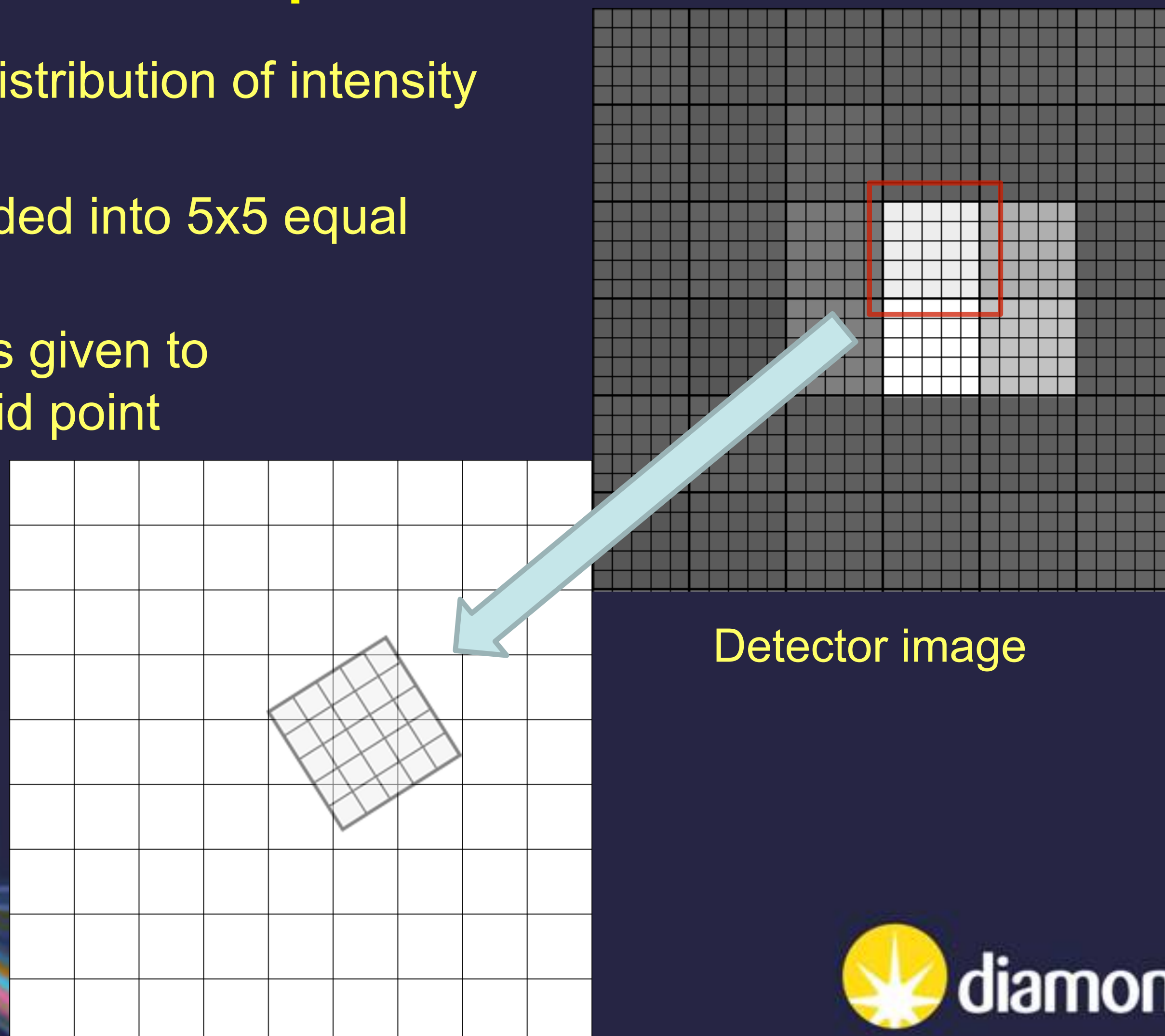
$$I_{v_3 j} = \int_{\Gamma_j \cap \Gamma_{v3}} \exp(-(\phi' - \phi)^2 / 2\sigma^2) d\phi'$$

- Fraction of intensity contributed by image frame, j to grid coordinate, v_3 is: $\frac{I_{v_3 j}}{I_j}$



Reciprocal space transform: gridding pixels

- Assumes flat distribution of intensity over pixel area
- Pixels sub-divided into 5x5 equal areas
- 1/25 intensity is given to transformed grid point



Detector image

Reciprocal space transform grid

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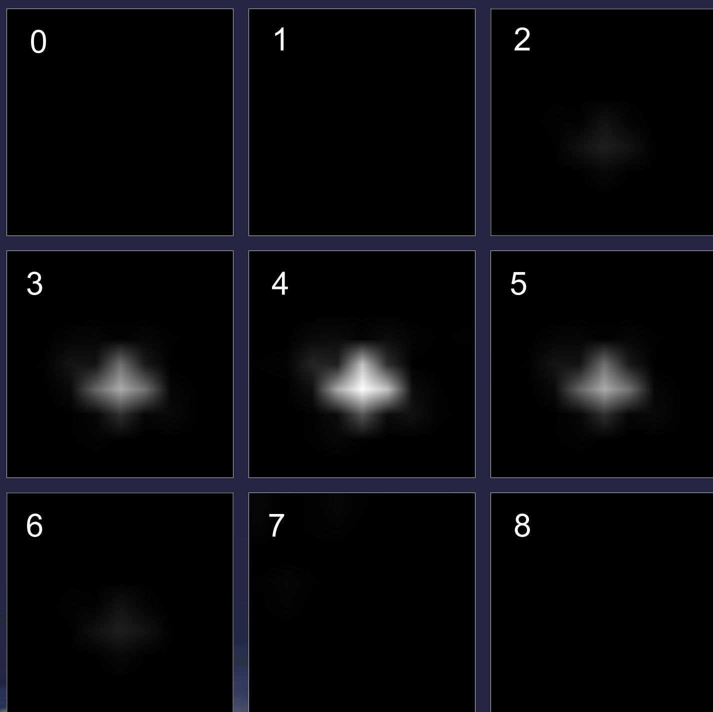
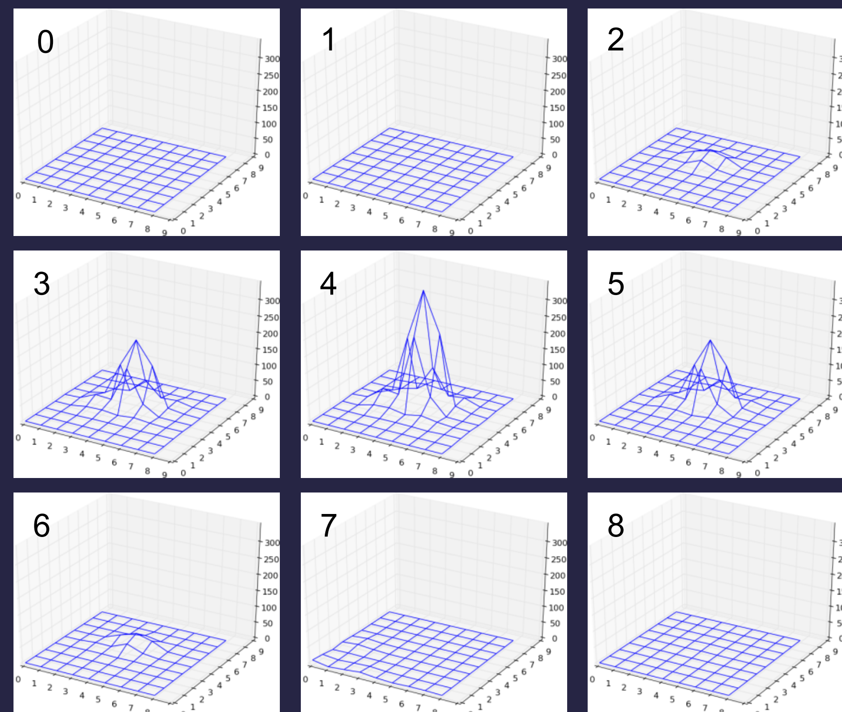
Transformed reflection profiles

2D



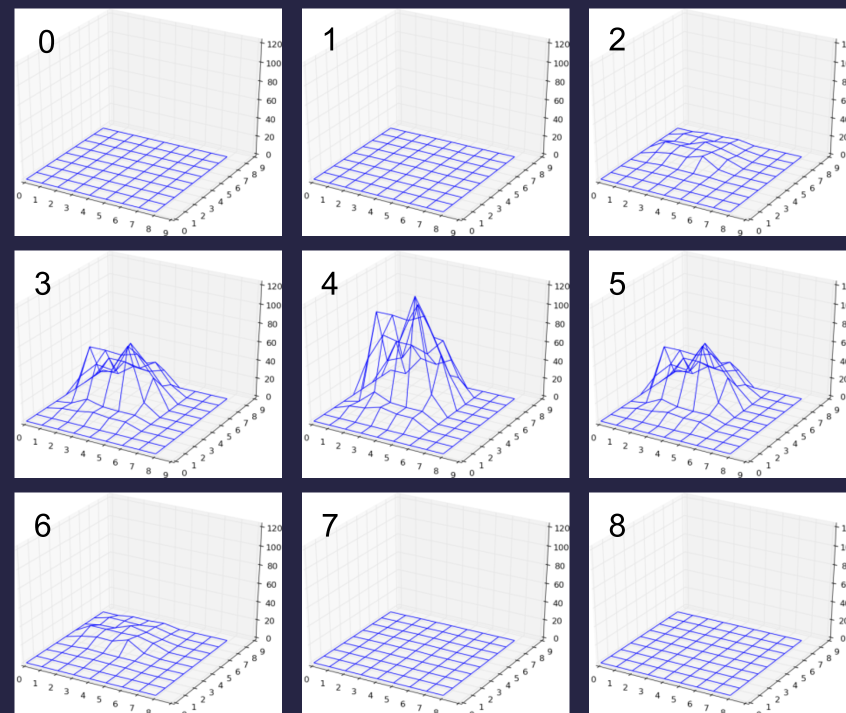
3D



Transformed reflection profiles

2D

3D



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Summary

- Implemented XDS algorithms for:
  - spot prediction
  - reflection mask calculation
  - background subtraction
  - reciprocal space transform

- Further work:
  - algorithms basically work but need to be rigorously tested
  - implementation of ‘missing’ XDS algorithms

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Questions?