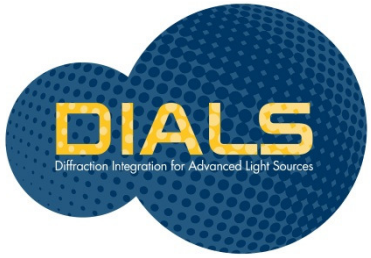
Centroid refinement

David Waterman

DIALS-4B



Topics

What is centroid refinement?

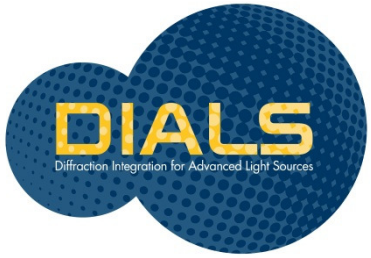
Refinement module overview

Parameterisation

Multi-panel detector

Scan-varying refinement

Model quality



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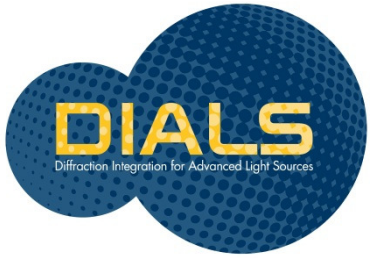
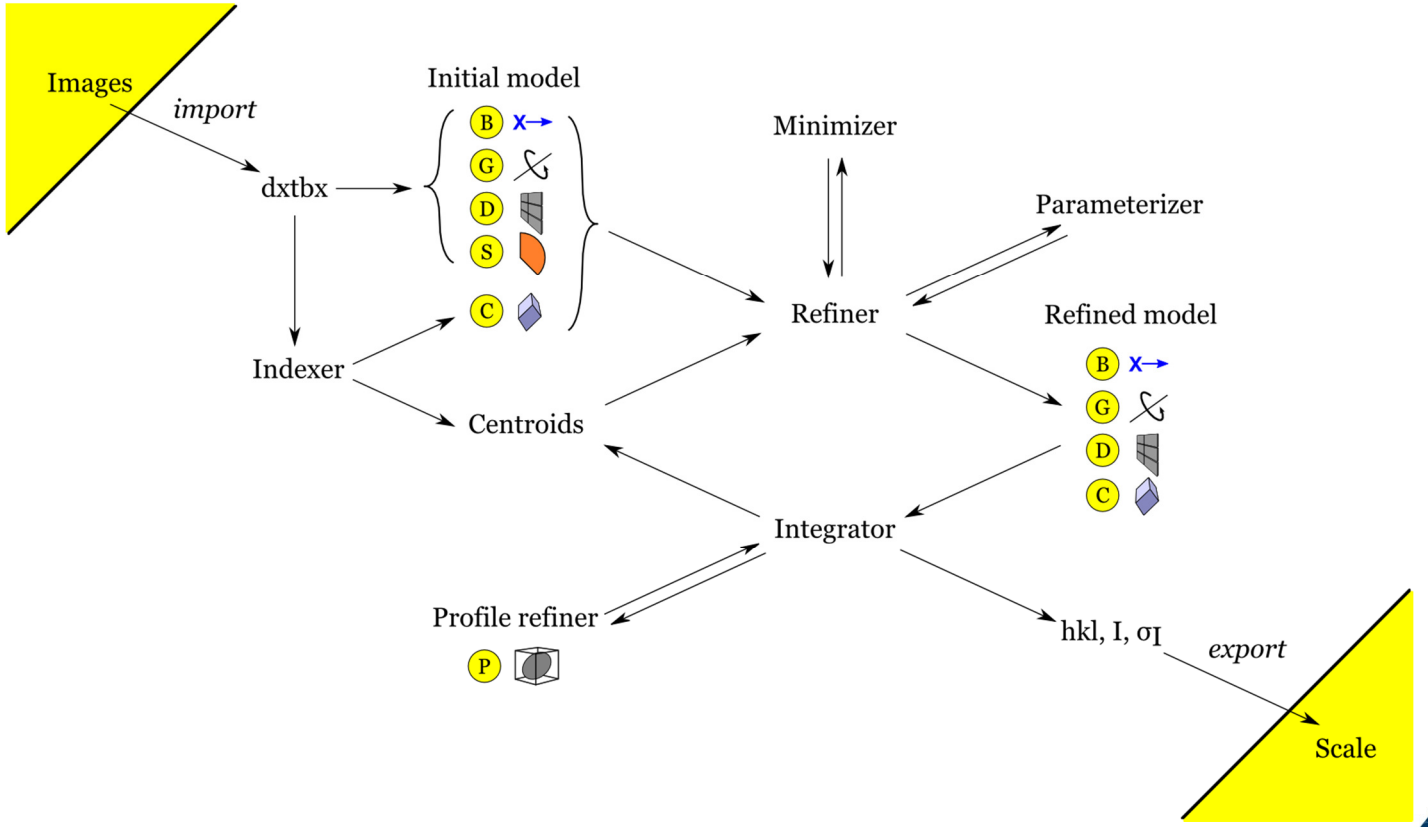


Centroid refinement

- Separation of ‘centroid refinement’ from profile formation / refinement
- Anatomy of rotation scan processing:



Centroid refinement

- In the terminology of the *EVAL* package*, we refine parameters that affect the *central impacts.*

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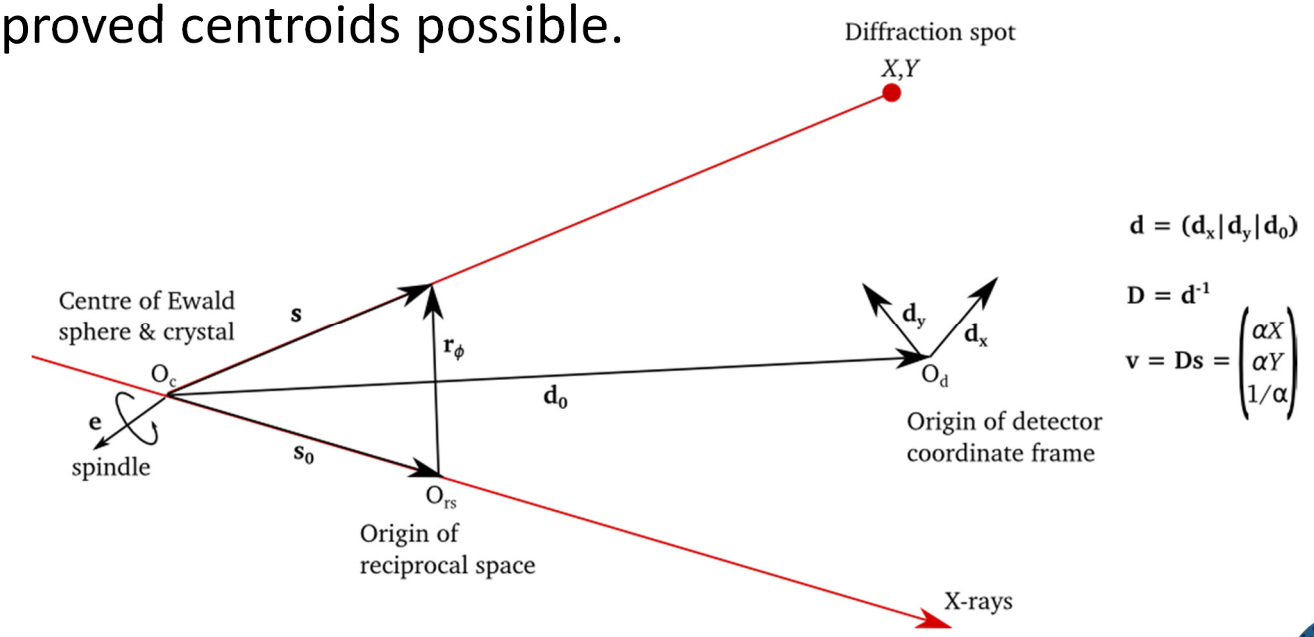
- Parameters that affect the *general impacts* (mosaicity, *Δλ,* …) are (to be) determined by separate 'profile refinement'.
- No profile model → no postrefinement, but second cycle with improved centroids possible.



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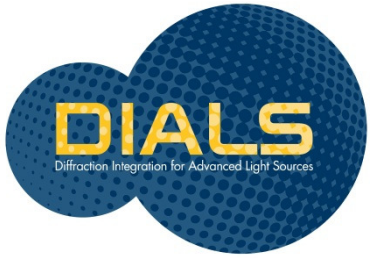
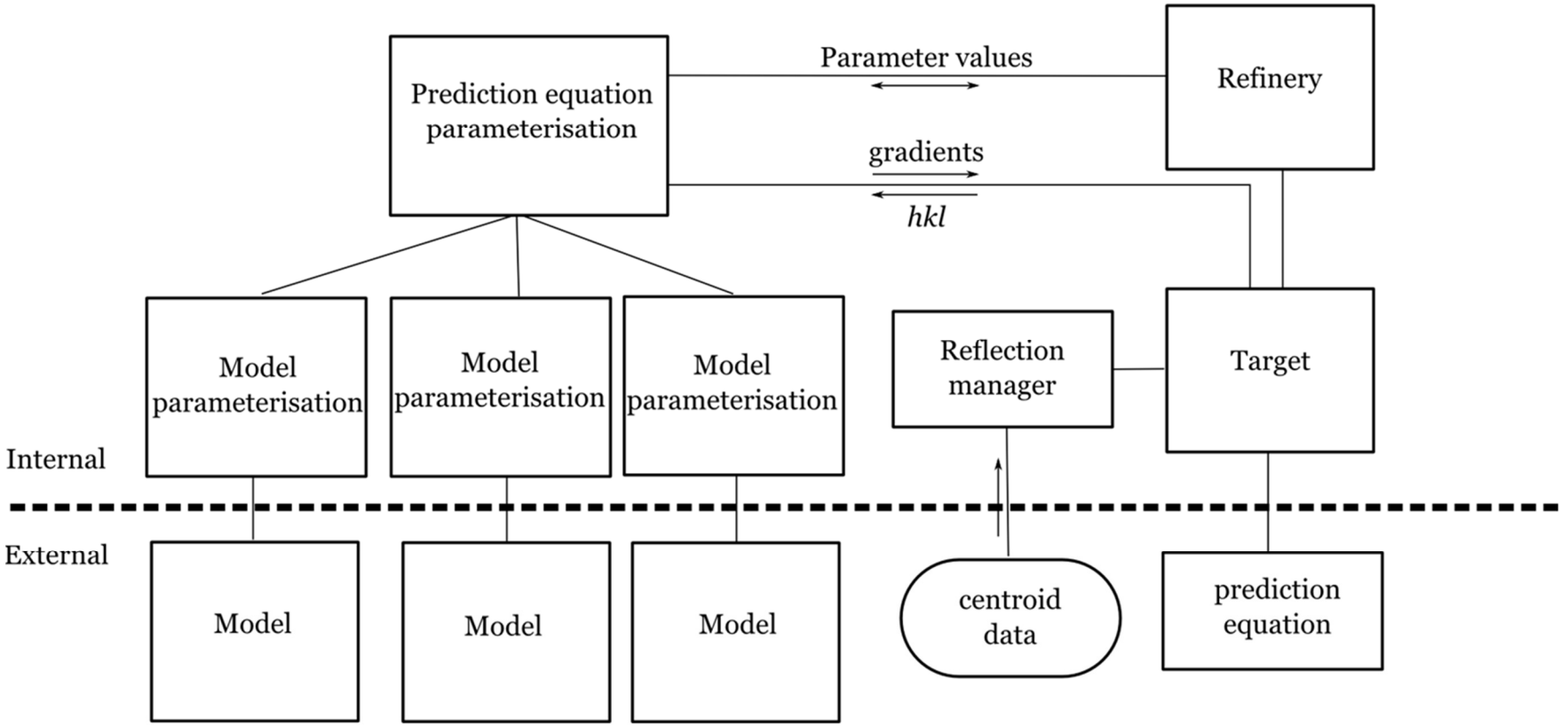


Overview



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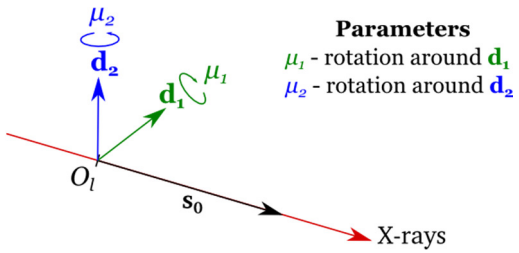
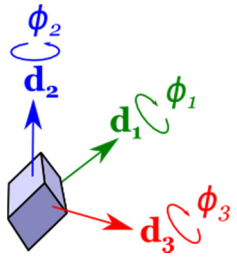
Overview

Parameterisation

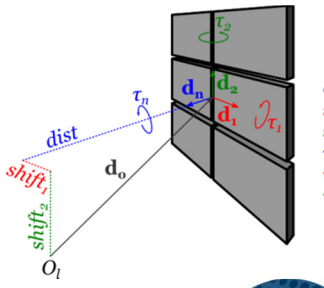
- Explicit separation of core abstract models from their parameterisations
- Encapsulate hardware- and experiment-specific parameterisation within a tuned refinement module
- Meanwhile DIALS models are shared throughout the program
- A basic parameterisation is provided, with 17 parameters for the triclinic case, for global refinement of the experiment geometry.
- Time-dependent evolution of the crystal model may be expressed by ‘checkpoints’ with a Gaussian smoother interpolation (adopting Phil Evans’ design from AIMLESS).



Parameters
μ_1 - rotation around $\mathbf{d}_1$
μ_2 - rotation around $\mathbf{d}_2$



Parameters
ϕ_1 - rotation around $\mathbf{d}_1$
ϕ_2 - rotation around $\mathbf{d}_2$
ϕ_3 - rotation around $\mathbf{d}_3$
$a, b, c, \alpha, \beta, \gamma$ - unit cell



Parameters
dist - detector distance along $\mathbf{d}_n$
shift$_1$ - translation in direction $\mathbf{d}_1$
shift$_2$ - translation in direction $\mathbf{d}_2$
τ_n - rotation around $\mathbf{d}_n \cong$ "roll"
τ_1 - rotation around $\mathbf{d}_1 \cong$"tilt"
τ_2 - rotation around $\mathbf{d}_2 \cong$"twist"

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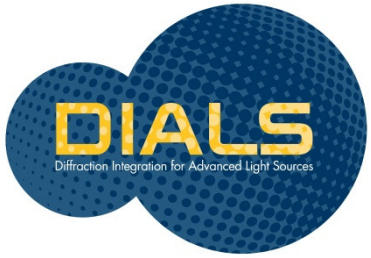
Overview

Global Refinement

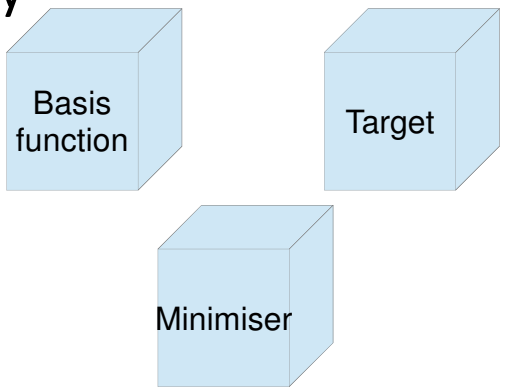
- Input diffraction spot indices, their centroids and estimated uncertainties (h, k, l; X, Y, ϕ; σ_X, σ_Y, σ_ϕ)
- Use all (useful) data available to refine a model to reduce RMSD of predicted centroids
- More physically meaningful:
  - Global refinement helps to recover from poorly determined parameters in local ϕ window
  - Avoids mopping up of effects by correlated parameters and therefore obtains realistic parameter values
- Global model allows for per-reflection parallelisation of integration



Overview

Modularity

- The refinement module is composed of 3 largely independent parts.
- This enables flexibility. In particular, a choice between two minimisation engines is provided: L-BFGS or Gauss Newton NLLS.
- Parameterisation is also modular. One default parameterisation is provided, but other versions could be written for specific situations.



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Overview

Proposed scheme for rotation scans

- A fully time invariant macrocycle to convergence to improve the detector and source models and define $\mathbf{U_0}$ and $\mathbf{B_0}$
- A macrocycle using scan-varying crystal parameterisations and static detector and source parameterisations
  - Parameters of the time dependent (Gaussian smoothed) models are restrained (tied) to the values that define $\mathbf{U_0}$ and $\mathbf{B_0}$
- Integration forms models for profiles, potentially improving the centroid positions
- Optionally repeat

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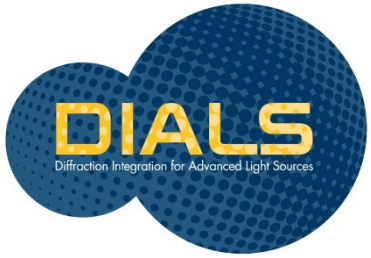
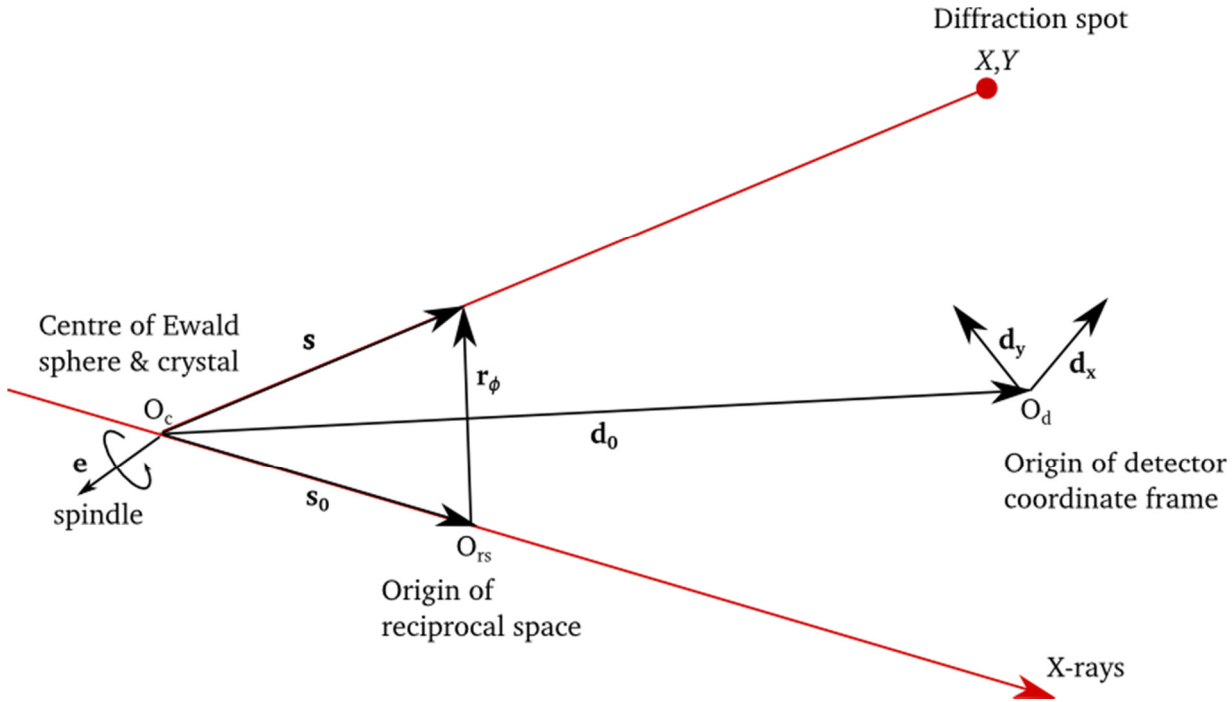
Model quality



Parameterisation

- The prediction equation comes from general, vectorial diffraction geometry



$$\mathbf{d} = (\mathbf{d}_x | \mathbf{d}_y | \mathbf{d}_0)$$

$$\mathbf{D} = \mathbf{d}^{-1}$$

$$\mathbf{v} = \mathbf{D}\mathbf{s} = \begin{pmatrix} \alpha X \\ \alpha Y \\ 1/\alpha \end{pmatrix}$$

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Parameterisation

For refinement we want at least the first derivatives of predicted centroids:

$$\frac{\partial \phi}{\partial p} = -\frac{\frac{\partial \mathbf{r}_\phi}{\partial p} \cdot \mathbf{s} + \mathbf{r}_\phi \cdot \frac{\partial \mathbf{s_0}}{\partial p}}{(\mathbf{e} \times \mathbf{r}_\phi) \cdot \mathbf{s_0}}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}p} = -\mathbf{D}\frac{\partial \mathbf{d}}{\partial p}\mathbf{v} + \mathbf{D}\left[\frac{\partial \mathbf{r}_\phi}{\partial p} + (\mathbf{e} \times \mathbf{r}_\phi)\frac{\partial \phi}{\partial p} + \frac{\partial \mathbf{s_0}}{\partial p}\right]$$

Neatly, these are factored into independent models:

$\frac{\partial \mathbf{d}}{\partial p}$	$\frac{\partial \mathbf{r}_\phi}{\partial p}$	$\frac{\partial \mathbf{s_0}}{\partial p}$
detector	crystal	beam direction

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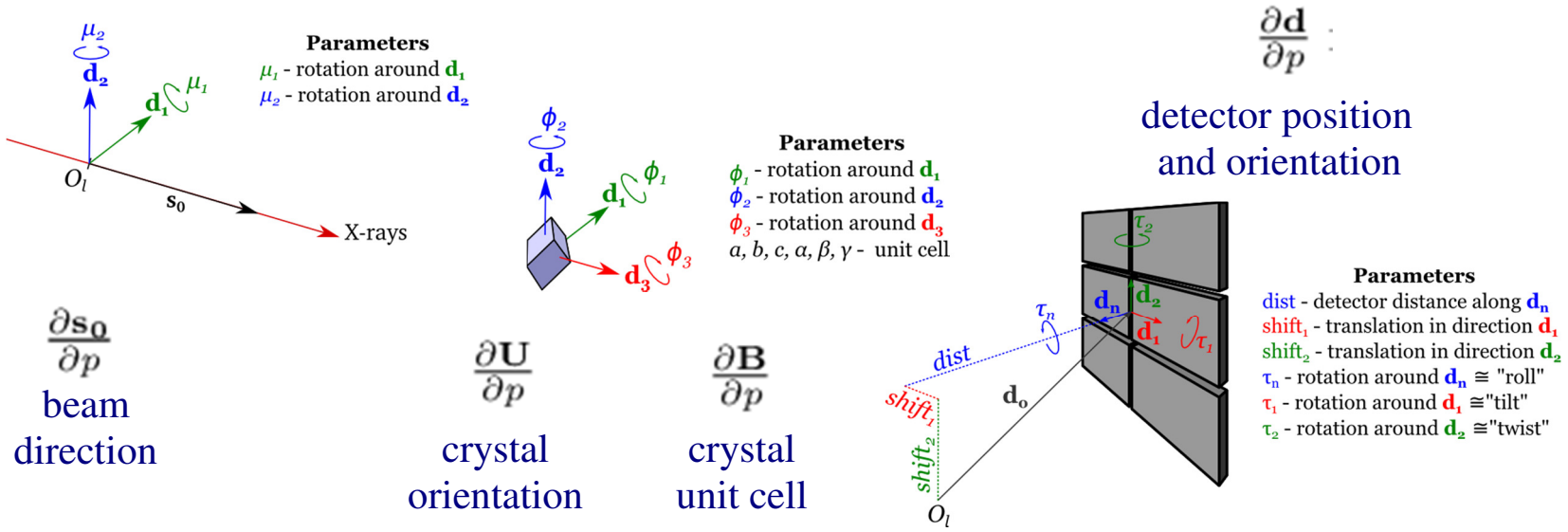
Parameterisation

- Each model parameterisation provides ∂[**state**]/∂p



- Separate PredictionParameterisation object takes ∂[**state**]/∂p for each model and converts to derivatives of *X*, *Y*, ϕ for each reflection
- Individual model parameterisations are encapsulated

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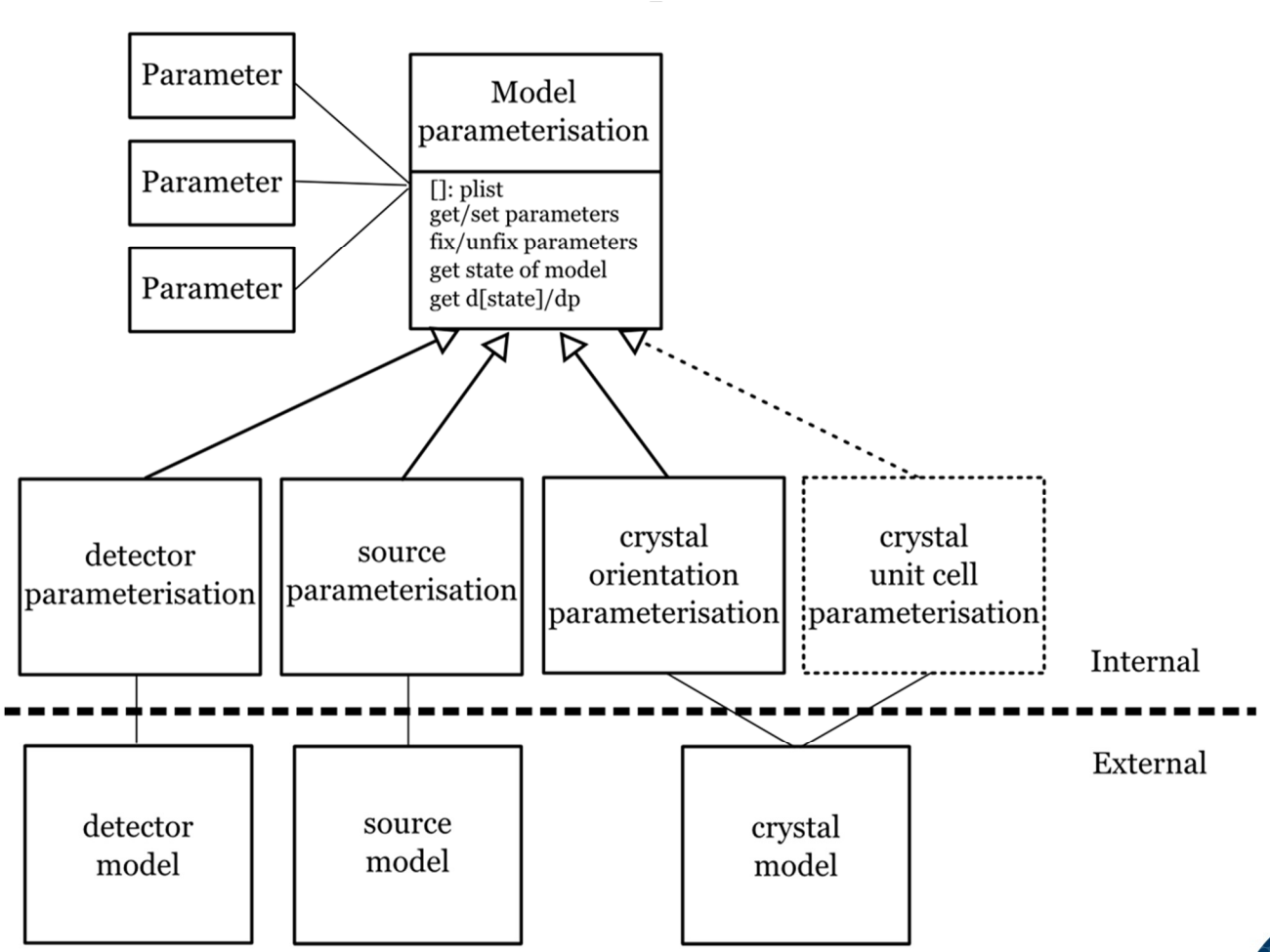
Parameterisation



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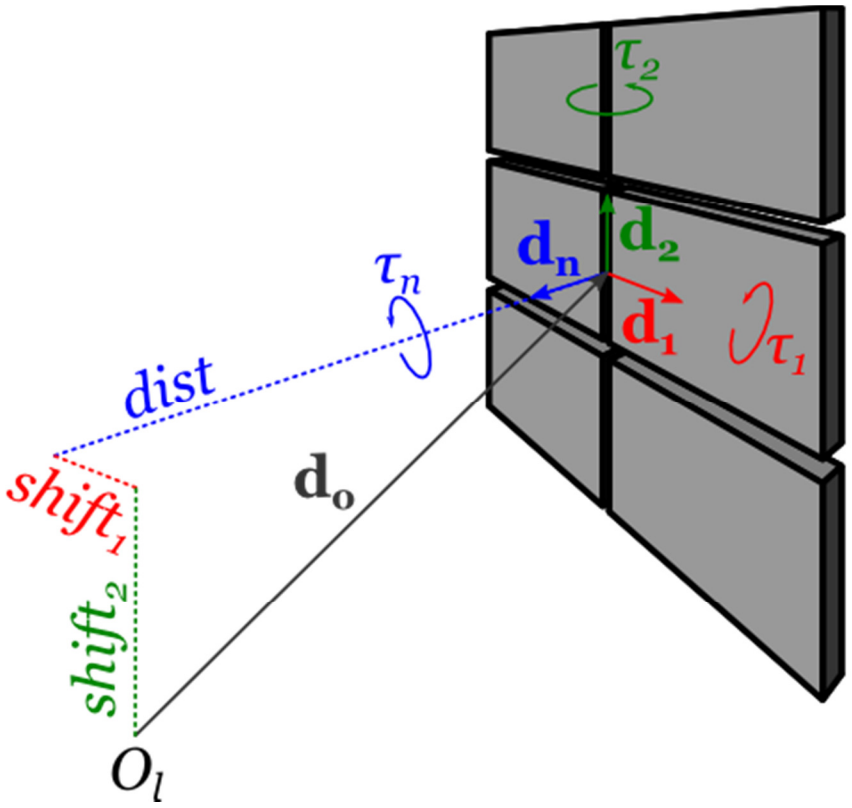
Parameterisation

A concrete example: detector parameterisation



Parameters

dist - detector distance along $\mathbf{d_n}$

$shift_1$ - translation in direction $\mathbf{d_1}$

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τ_n - rotation around $\mathbf{d_n}$ ≅ "roll"

τ_1 - rotation around $\mathbf{d_1}$ ≅"tilt"

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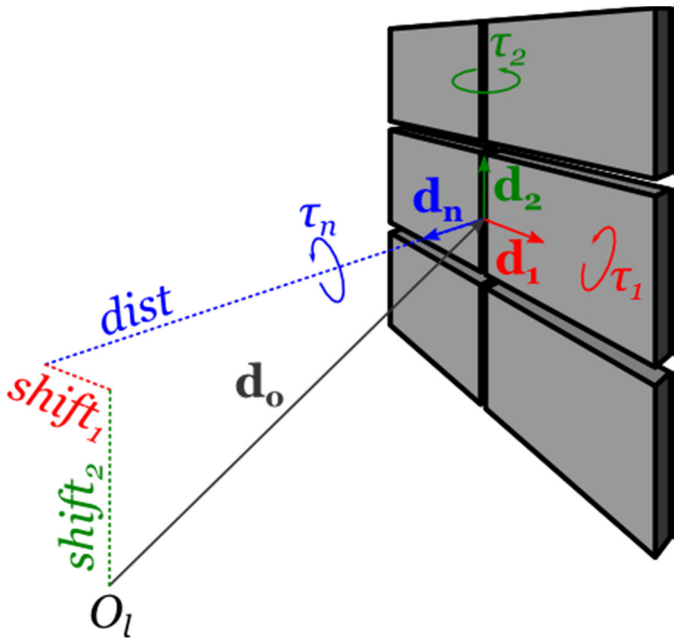
Parameterisation

- Initial sensor matrix provides $\mathbf{d_0}$, $\mathbf{d_1}$, $\mathbf{d_2}$, $\mathbf{d_n}$. NB here $\mathbf{d_0}$ is chosen to meet the centre of the detector, not the corner
- Translation parameters are immediately *dist* along $\mathbf{d_n}$ and $shift_1$, $shift_2$ along $\mathbf{d_1}$, $\mathbf{d_2}$
- Initial rotation angles all 0.0, around axes $\mathbf{d_1}$, $\mathbf{d_2}$, $\mathbf{d_n}$



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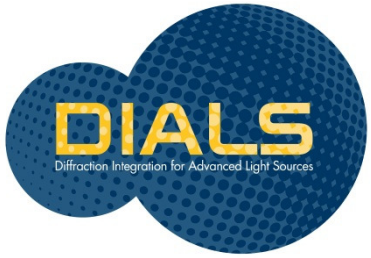
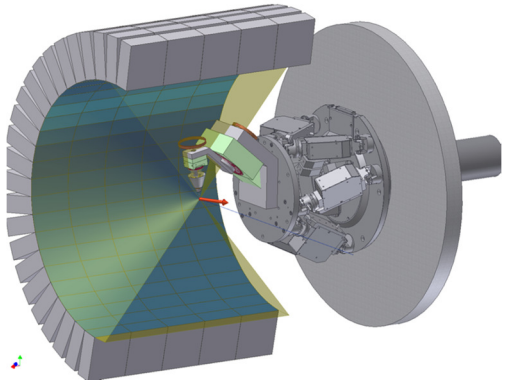


Multi-panel detector

- A small extension of the default parameterisation accommodates refinement of multi-tile detectors as one rigid unit
- Each sensor panel *k* has its own matrix $\mathbf{d}^k = (\mathbf{d_x}^k | \mathbf{d_y}^k | \mathbf{d_0}^k)$
- These vectors are linear combinations of $\mathbf{d_0}$ and the local coordinate system $\mathbf{d_1}$, $\mathbf{d_2}$, $\mathbf{d_n}$ that moves with the detector:

$$\mathbf{d}_x^k = \alpha_1^k \mathbf{d_1} + \alpha_2^k \mathbf{d_2} + \alpha_3^k \mathbf{d_n}$$
$$\mathbf{d}_y^k = \beta_1^k \mathbf{d_1} + \beta_2^k \mathbf{d_2} + \beta_3^k \mathbf{d_n}$$
$$\mathbf{d}_0^k = \mathbf{d_0} + \gamma_1^k \mathbf{d_1} + \gamma_2^k \mathbf{d_2} + \gamma_3^k \mathbf{d_n}$$



- Thus the derivatives $\partial\mathbf{d}^k/\partial p$ for each sensor are easily calculated by linear combinations of $\partial\mathbf{d_o}/\partial p$, $\partial\mathbf{d_1}/\partial p$, $\partial\mathbf{d_2}/\partial p$ and $\partial\mathbf{d_n}/\partial p$

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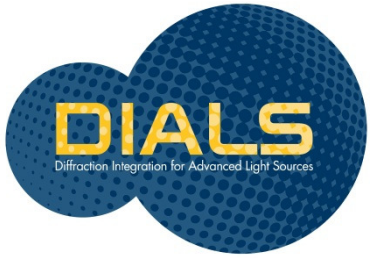
Multi-panel detector

- In practice, this required some changes in refinement to ensure:
  - The panel number of observations is tracked
  - Prediction is then done for specific panels
  - Multi-state parameterisations are possible
  - A few tweaks: set rmsd cutoffs after querying pixel size of every panel, choose a panel to be the reference for the coordinate frame, choose single/multi parameterisation automatically, ...
- Multi-panel parameterisation tested:
  - By creating a 3×3 array filling the same space as a single panel and ensuring refinement proceeds identically
  - By comparing all derivatives with finite difference estimates, including the general case of non-coplanar panels
  - By refining real data with detectors created by the FormatCBFMiniPilatus and FormatCBFMiniPilatusSplit6M classes and ensuring these give the same results
- DIALS refinement now handles single/multi panel detector automatically



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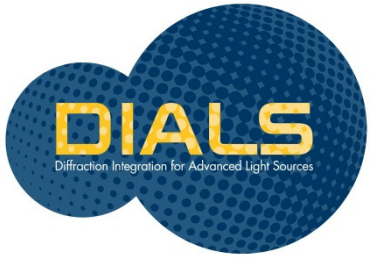
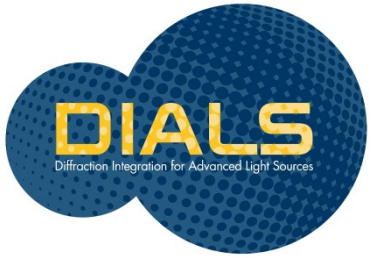


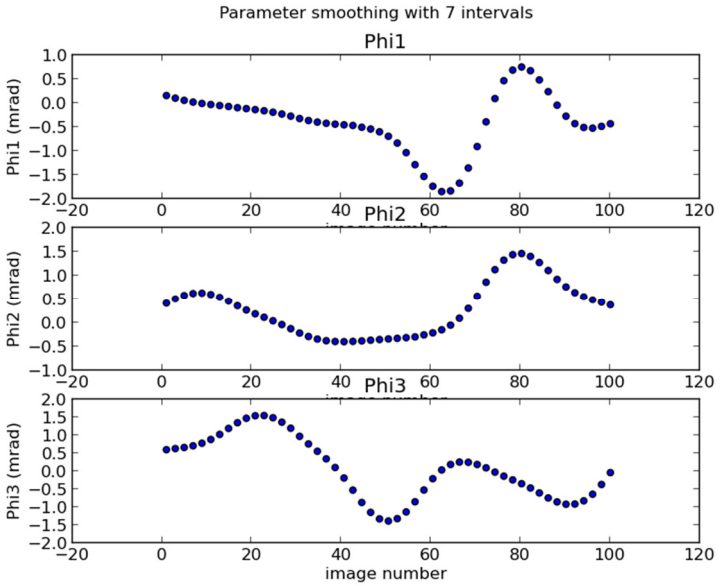
Scan-varying refinement

- For rotation scans we are interested in time- or dose-dependent evolution of the crystal model
- Image number of reflection centroid is a proxy for time or dose. It is something we can measure from the images
- Use this as the independent axis, hence ‘scan-varying’
- We assert that no crystal parameter has a discontinuity during a properly recorded rotation scan
- AIMLESS models time-dependent parameters using a simple Gaussian smoother. Let’s try this for DIALS



Scan-varying refinement

- Implemented Gaussian smoother from Aimless
- Derivatives ∂**U**(*t*)/∂p and ∂**B**(*t*)/∂p tested by FD for crystal orientation and unit cell parameters
- There are three adjustable variable for the smoother
  - number of samples in total
  - sigma
  - number of samples to average
- How do we know what values are appropriate?



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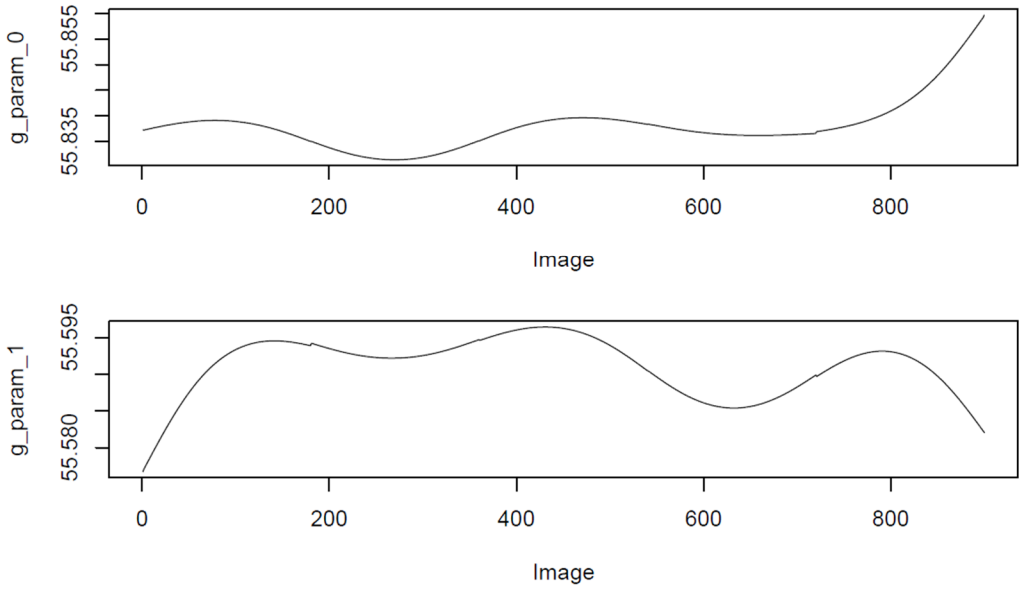
Scan-varying refinement

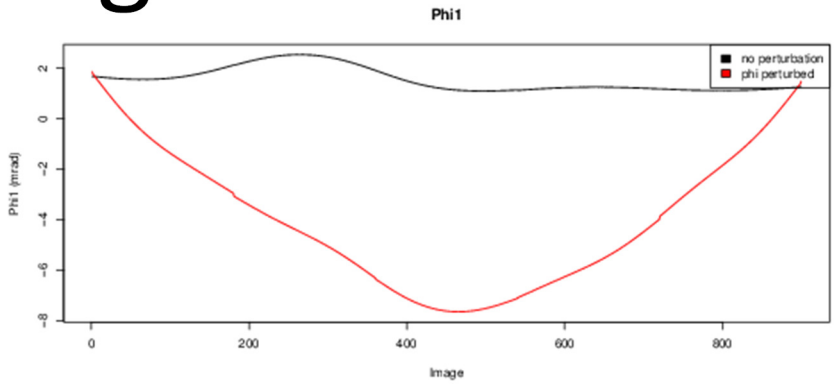
- This is now an available in DIALS refinement (though still without restraints to $\mathbf{U_0}$ and $\mathbf{B_0}$)
- Globally smoothed model avoids discontinuities between batch jobs (*cf*. MOSFLM, XDS) that have their own local refinement
- Requires new algorithm for prediction of all reflections post refinement
- All used in dials.process. More tests needed esp. with bad data

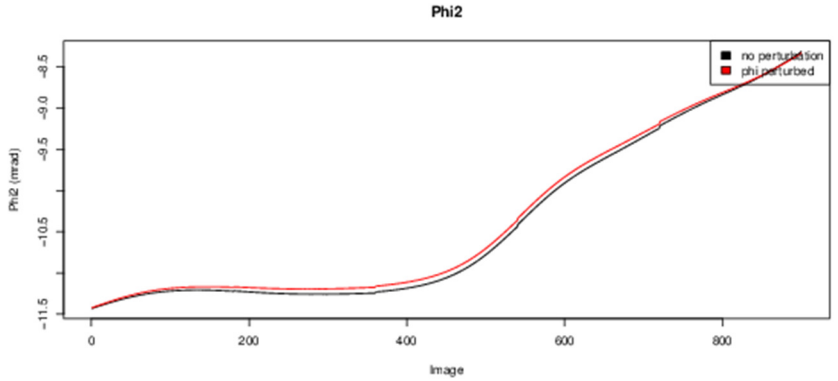


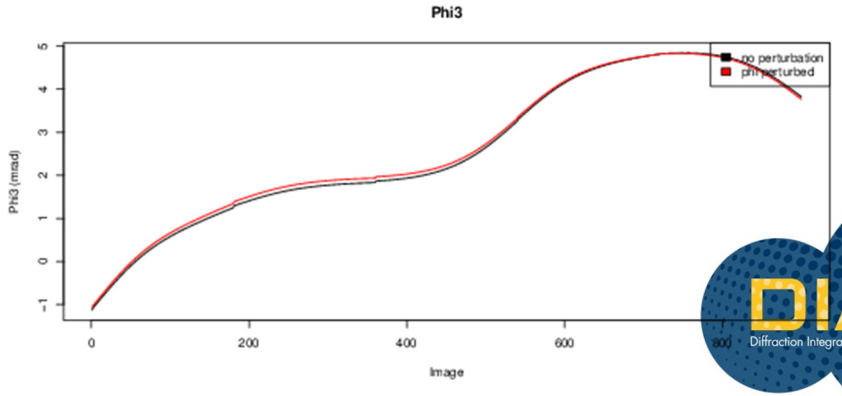
Scan-varying refinement

Proof of principle test

- Apply sinusoidal perturbation to reflecting phi, peaking at +0.5 degrees
- Refine, and compare crystal orientation parameters over the scan







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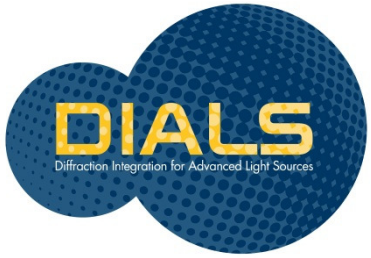
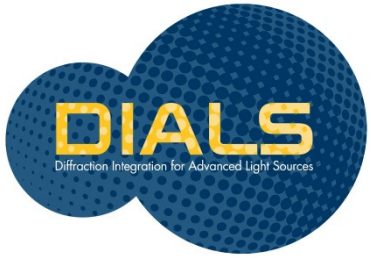


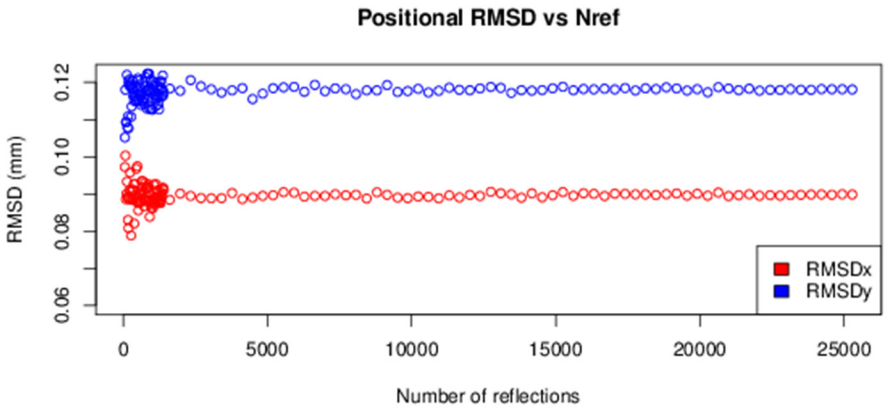
Model quality

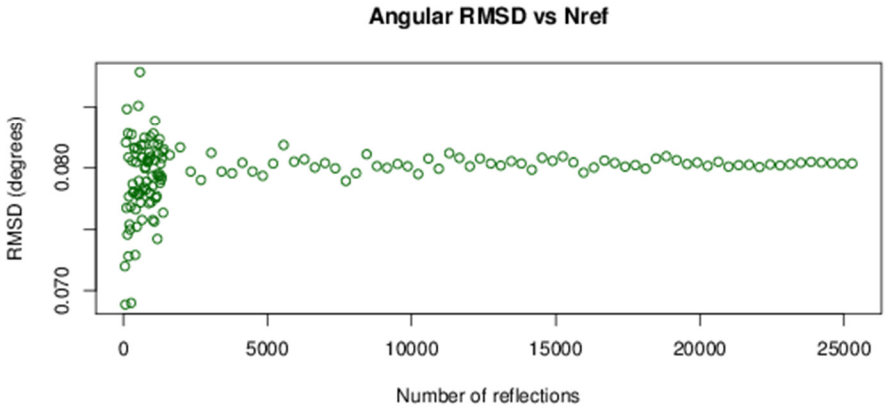
- How many reflections are needed for refinement?
- Explore with a good dataset
  - `dials_regression/centroid_test_data`
  - 180° sweep, P 4
  - 29’000 “strong” reflections written to SPOT_ALL.XDS
  - Refinement performed with a ‘regularized’ model, i.e. known to be wrong



Model quality

- By default refinement samples 50 reflections per degree of the scan
- Perhaps we can usually “get away with” using far fewer?
- Need to do this test with scan-varying refinement on a dataset where it matters





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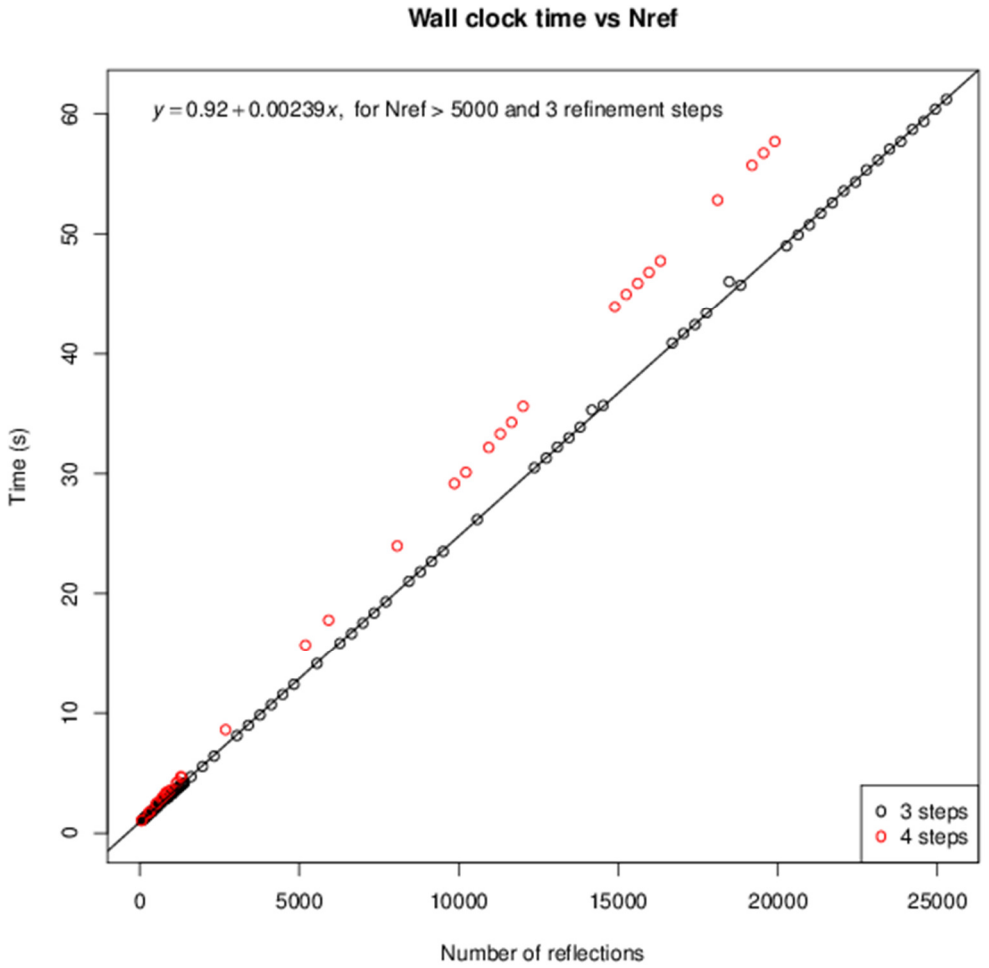
Model quality

- Execution time scales linearly with Nref, with only a small constant overhead



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