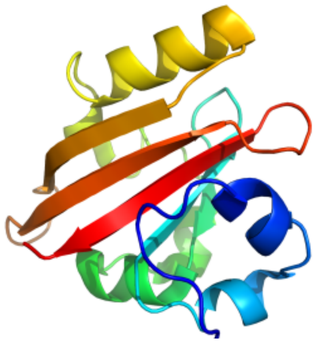
Millepede-II for photon science

Borrowing HEP algorithms for detector alignment
with serial crystallography data



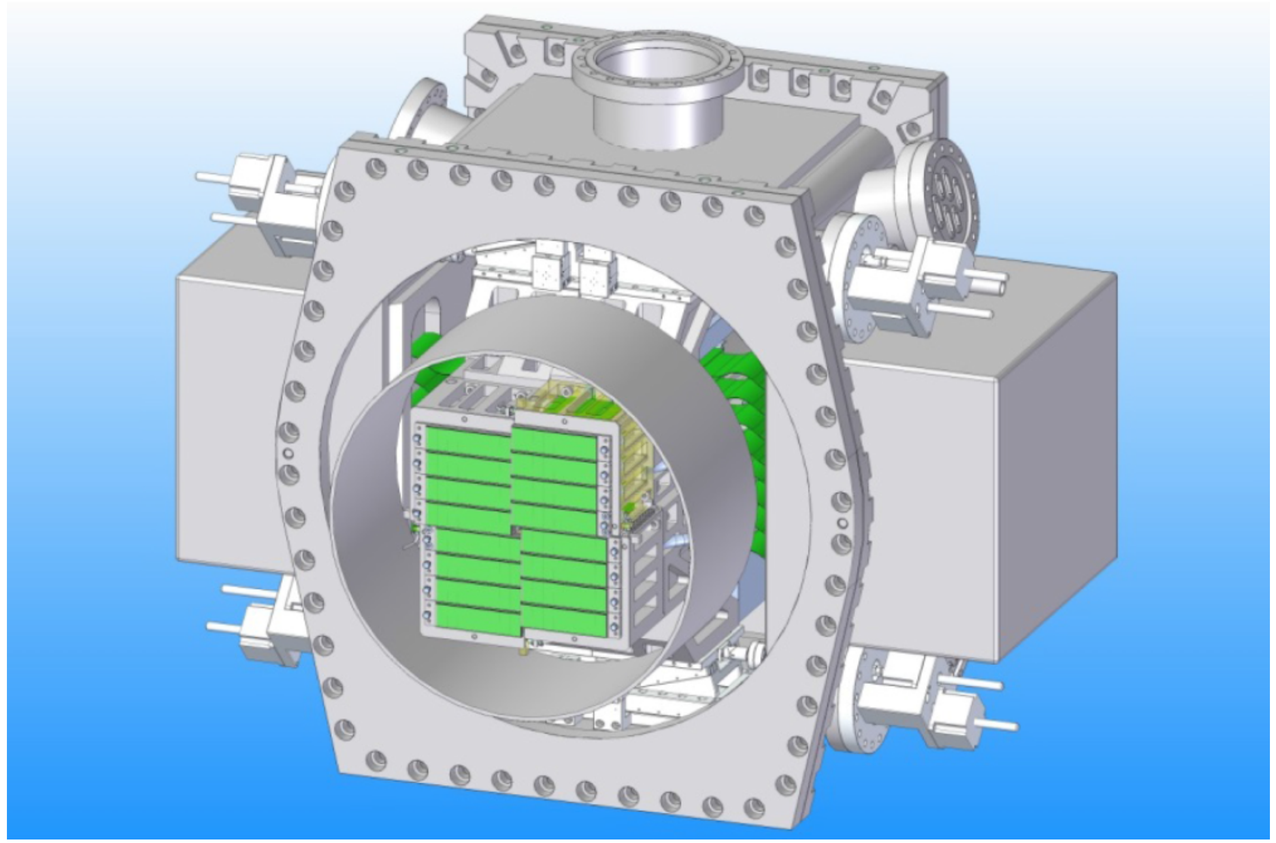
Thomas White
DESY Photon Science Computing Workshop
10 Nov 2023

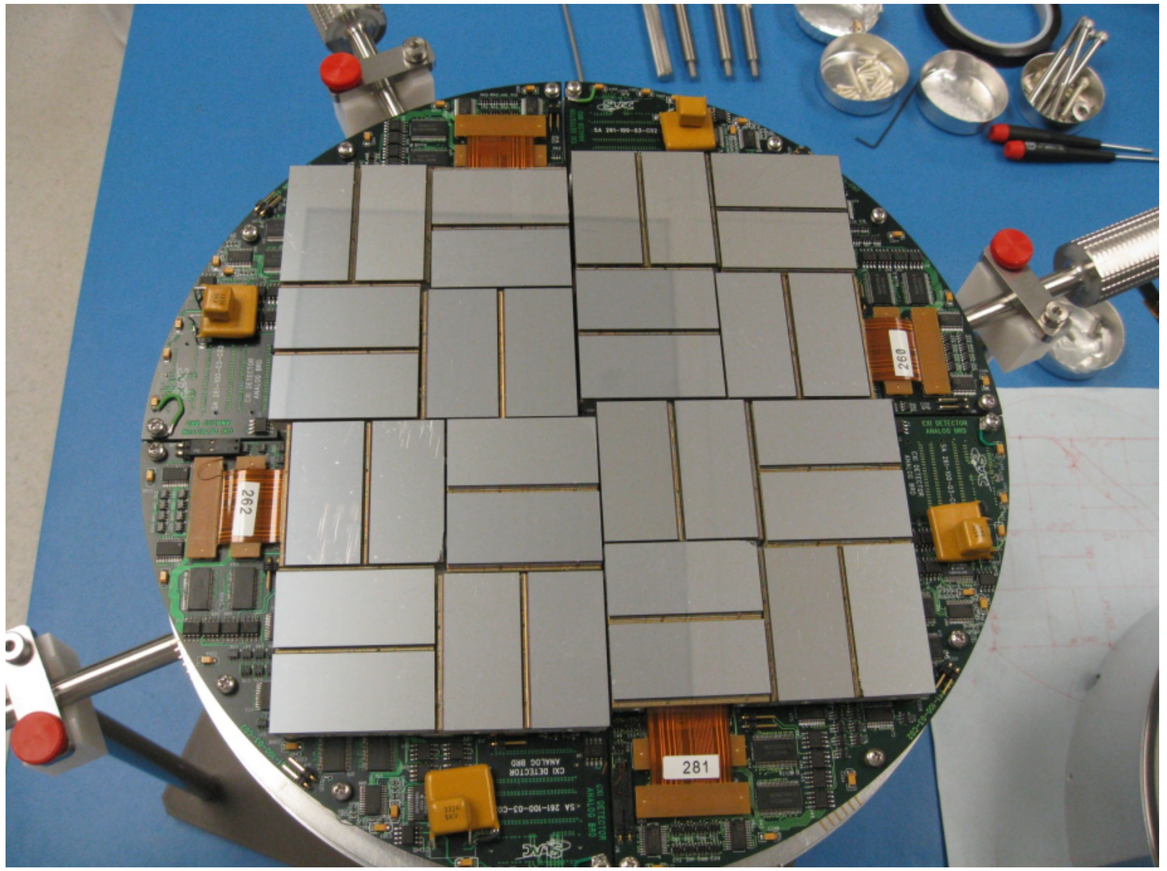
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

Detector geometry in serial crystallography

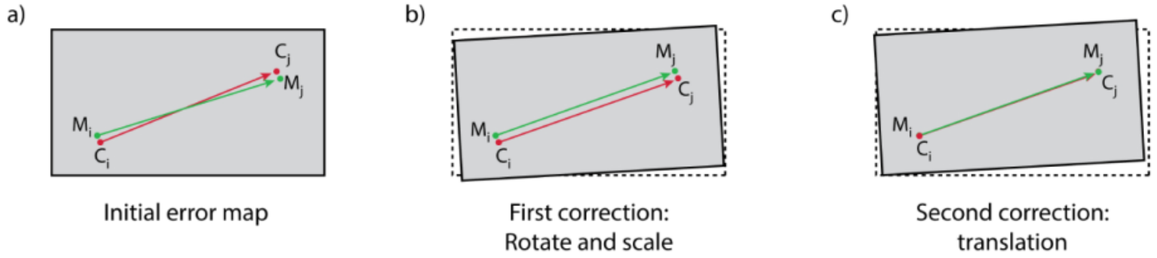
Data analysis in serial crystallography relies on accurate detector geometry



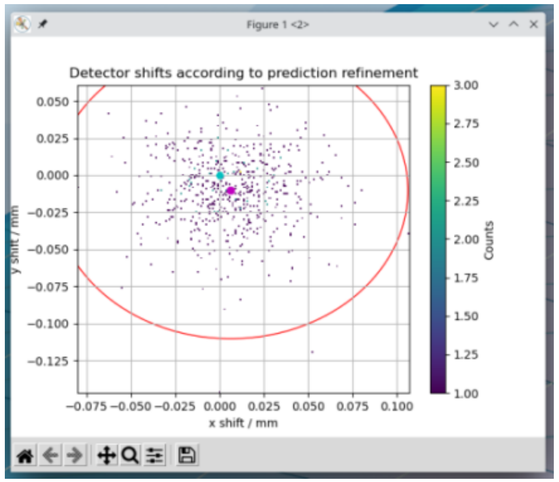


Multi-panel detectors: mostly for XFELs, but coming to a synchrotron beamline near you soon....

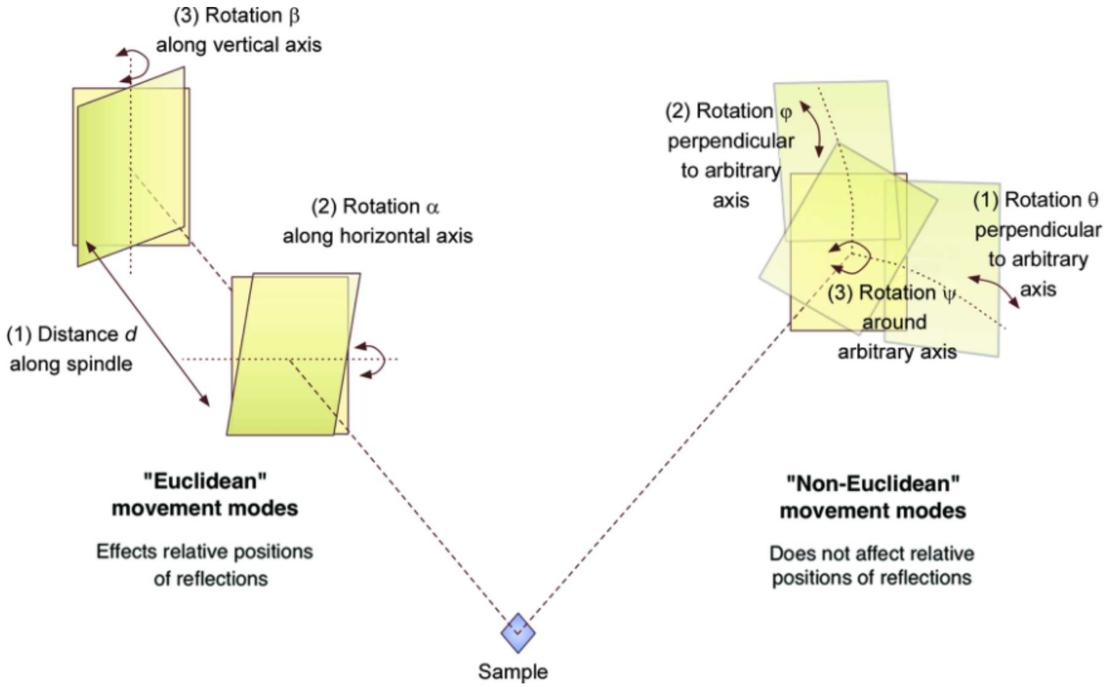
Algorithms for detector geometry refinement



Yefanov, Optics Express 23 (2015) p28459
"geoptimiser" algorithm: Convert peak-reflection offsets to geometry corrections, and take mean.



Prediction refinement/"detector-shift" (in CrystFEL)
Refine offsets+cell parameters for each pattern, and take the mean of the detector offset distributions



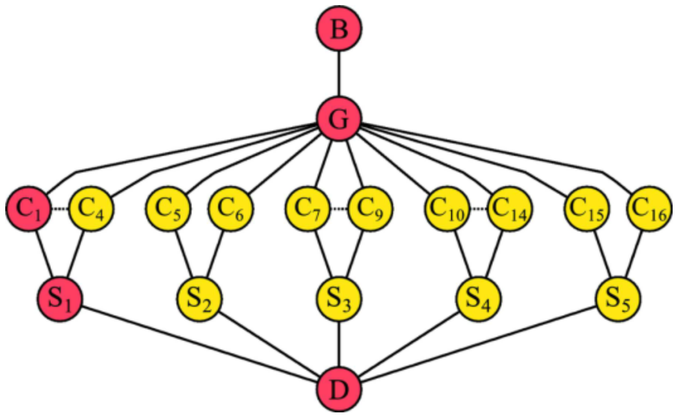
Ginn (2017), J. Sync. Rad. 24, p1152
"Slip and slide" algorithm: Nelder-Mead minimisation with careful parameterisation, iterative between cell and geometry

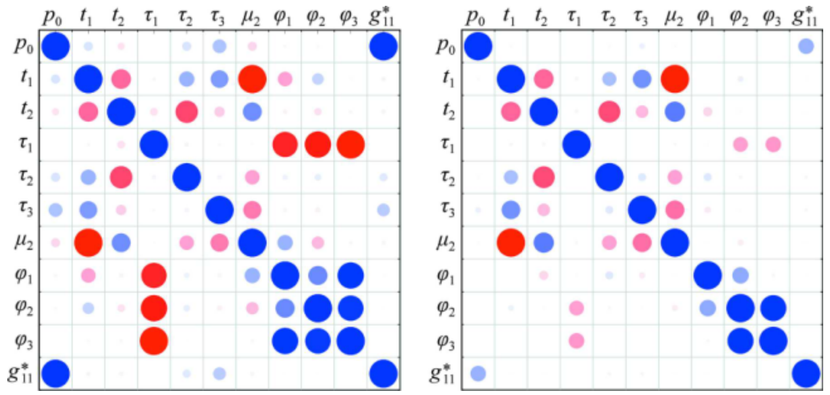
+several others

Current state of the art (my opinion)

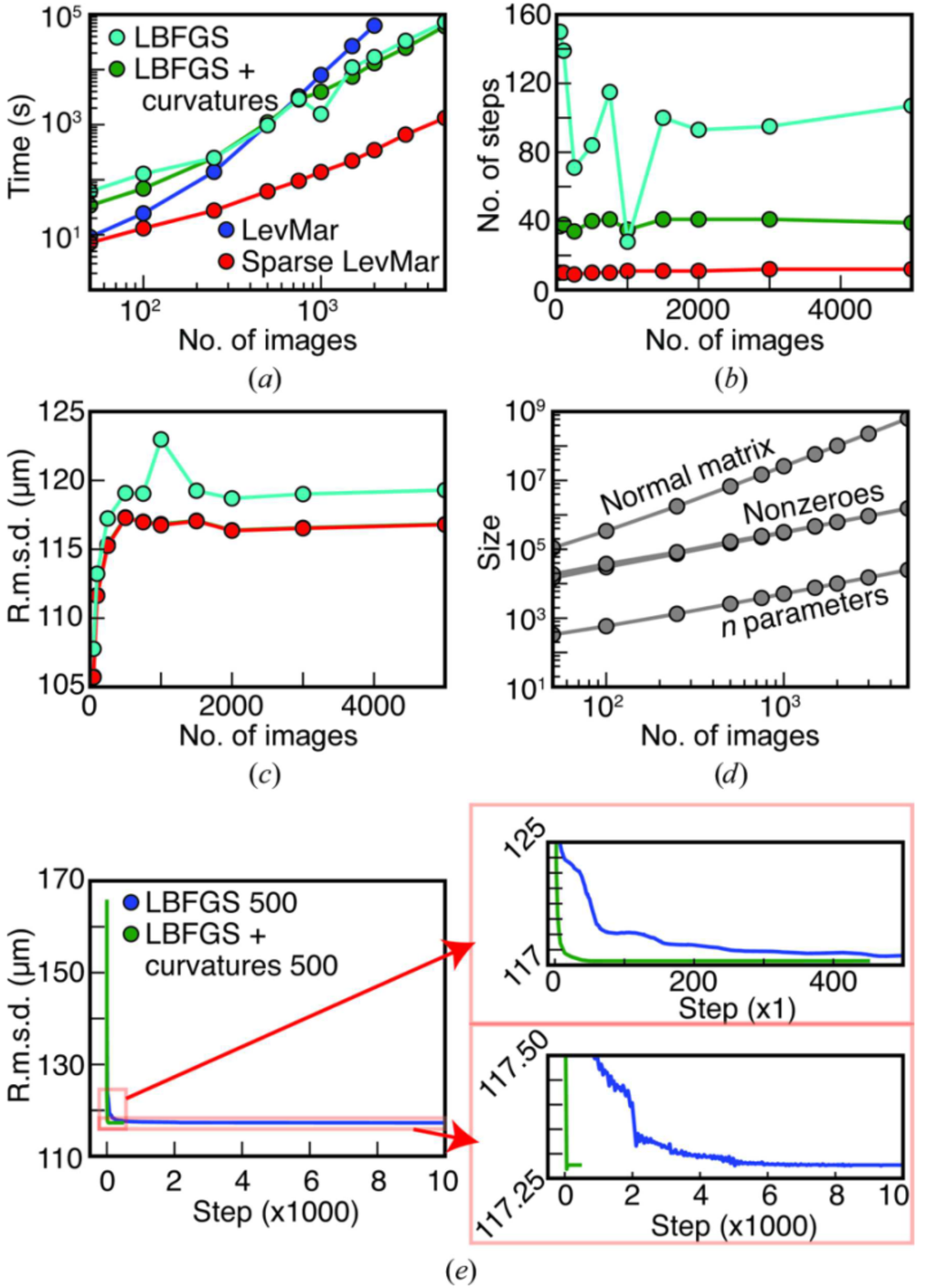
Brewster, Acta Cryst. D74 (2018) p877
+ Waterman, Acta Cryst. D72 (2016) p558

DIALS geometry refinement:
One detector geometry model, many crystal models





"Just make the big matrix and get on with solving it"



The "Millepede principle"

$$\left(\begin{array}{c|ccc} \boldsymbol{C} & \cdots & \boldsymbol{H}_k & \cdots \\ \hline \cdots & \cdots & \mathbf{0} & \mathbf{0} \\ \boldsymbol{H}_k^{\mathrm{T}} & \mathbf{0} & \boldsymbol{C}_k^{\mathrm{track}} & \mathbf{0} \\ \cdots & \mathbf{0} & \mathbf{0} & \cdots \end{array}\right) \times \left(\begin{array}{c} \boldsymbol{\Delta p} \\ \hline \cdots \\ \Delta \boldsymbol{q}_k^{\mathrm{track}} \\ \cdots \end{array}\right) = \left(\begin{array}{c} \boldsymbol{b} \\ \hline \cdots \\ \boldsymbol{b}_k^{\mathrm{track}} \\ \cdots \end{array}\right) \qquad k = \text{ track index}$$

The magic part:

$$\boldsymbol{C} := \boldsymbol{C} + \sum_i w_i \boldsymbol{d}_i^{\mathrm{global}} \left(\boldsymbol{d}_i^{\mathrm{global}}\right)^{\mathrm{T}} \qquad \boldsymbol{b} := \boldsymbol{b} + \sum_i w_i r_i \boldsymbol{d}_i^{\mathrm{global}} \qquad \boldsymbol{H}_k = \sum_i w_i \boldsymbol{d}_i^{\mathrm{global}} \left(\boldsymbol{\delta}_i^{\mathrm{local}}\right)^{\mathrm{T}}$$

and finally for the track $\boldsymbol{C} := \boldsymbol{C} - \boldsymbol{H}_k \boldsymbol{V}_k \boldsymbol{H}_k^T \qquad \boldsymbol{b} := \boldsymbol{b} - \boldsymbol{H}_k \left(\boldsymbol{V}_k \boldsymbol{b}_k\right)$

The 'blue' equations transfer the 'local' information to the global parameters.

After the loop on all tracks the complete information is collected; now the matrix equation for the global parameters has to be solved:

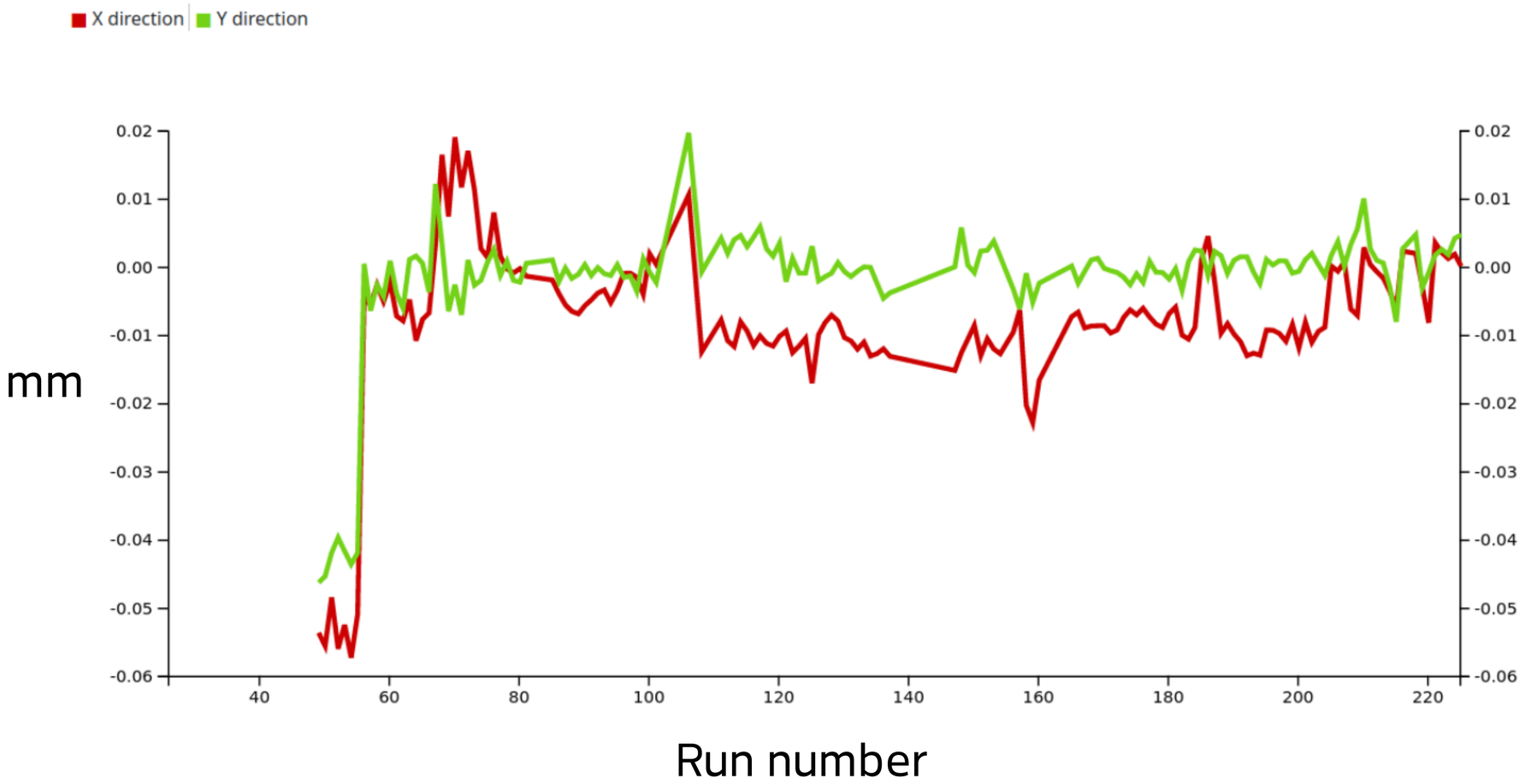
solve $\boldsymbol{C} \Delta \boldsymbol{p}^{\mathrm{global}} = \boldsymbol{b}$ for $\Delta \boldsymbol{p}^{\mathrm{global}}$ e.g. by $\Delta \boldsymbol{p}^{\mathrm{global}} = \boldsymbol{C}^{-1}\, \boldsymbol{b}$

Note: matrices $\boldsymbol{C}$ and vectors $\boldsymbol{b}$ from several data sets can be simply added to get combined result.

Blobel, ATLAS Inner Detector Alignment and Commissioning Workshop, Ringberg, June 2006
Shamelessly stolen from https://www.desy.de/~sschmitt/blobel/ATLASalign.pdf

Millepede-II being used in CrystFEL

"align_detector" in recent (development/Git) versions of CrystFEL
Used at P11 as part of real-time pipeline ("easy" case):



Work ongoing: better parameterisation, control of "weak modes" and more.

Other "Millepede problems"?

→ One protein model, many conformational states?

→ One set of combined structure factors, many partial data sets (post-refinement)?

→ Any calibration problem, not just geometry?

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