Playing with XDS predictions (using Numpy)

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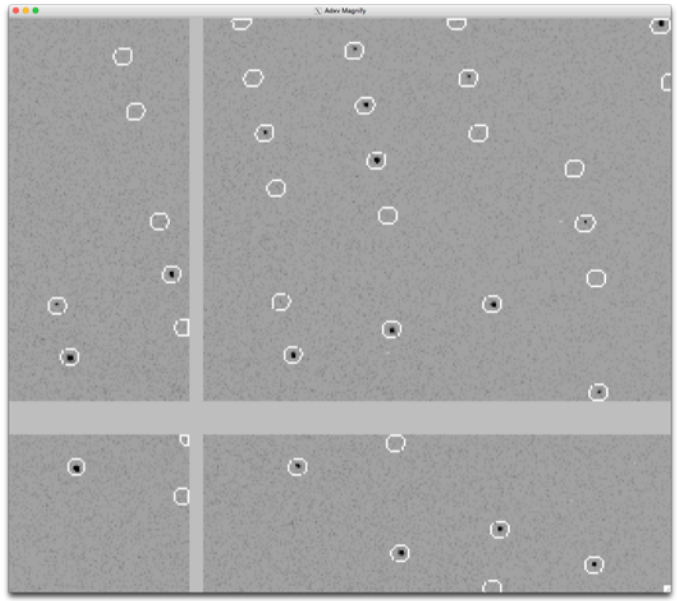
Seeing predictions when using XDS

- In data processing, it is extremely important to see if prediction matches actual spot positions
- In XDS, FRAME.cbf is provided to check the predictions on the last integrated frame

FRAME.cbf
(displayed with Adxv)



- What if we want to see predictions on an arbitrary frame?
  - Run INTEGRATE for the specific frame
- Alternative way: **calculate predictions by ourselves** based on XPARM.XDS (indexing result)
  ..because this is Computing School.

Tools used in this tutorial

- Python2.7 with CCTBX and Numpy (1.8 or higher)
  - If you have phenix or ccp4, you may use `phenix.python` or `ccp4-python` (with phenix-1.10 or ccp4-7.0)
- XDS
- generate_XDS.INP
- Adxv

Slides, links, and source code are available on the Github

https://github.com/keitaroyam/ECACOMSIG-ECM30

Short URL: http://git.io/v6zbx

Reference paper

Acta Cryst. (2010). D**66**, 133–144. doi:10.1107/S0907444909047374

research papers

Acta Crystallographica Section D
Biological Crystallography
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Integration, scaling, space-group assignment and post-refinement

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Important steps in the processing of rotation data are described that are common to most software packages. These programs differ in the details and in the methods implemented to carry out the tasks. Here, the working principles underlying the data-reduction package *XDS* are explained, including the new features of automatic determination of spot size and reflecting range, recognition and assignment of crystal symmetry and a highly efficient algorithm for the determination of correction/scaling factors.

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A version of this paper will be published as a chapter in the new edition of Volume *F* of *International Tables for Crystallography*.

Related sections in this tutorial:

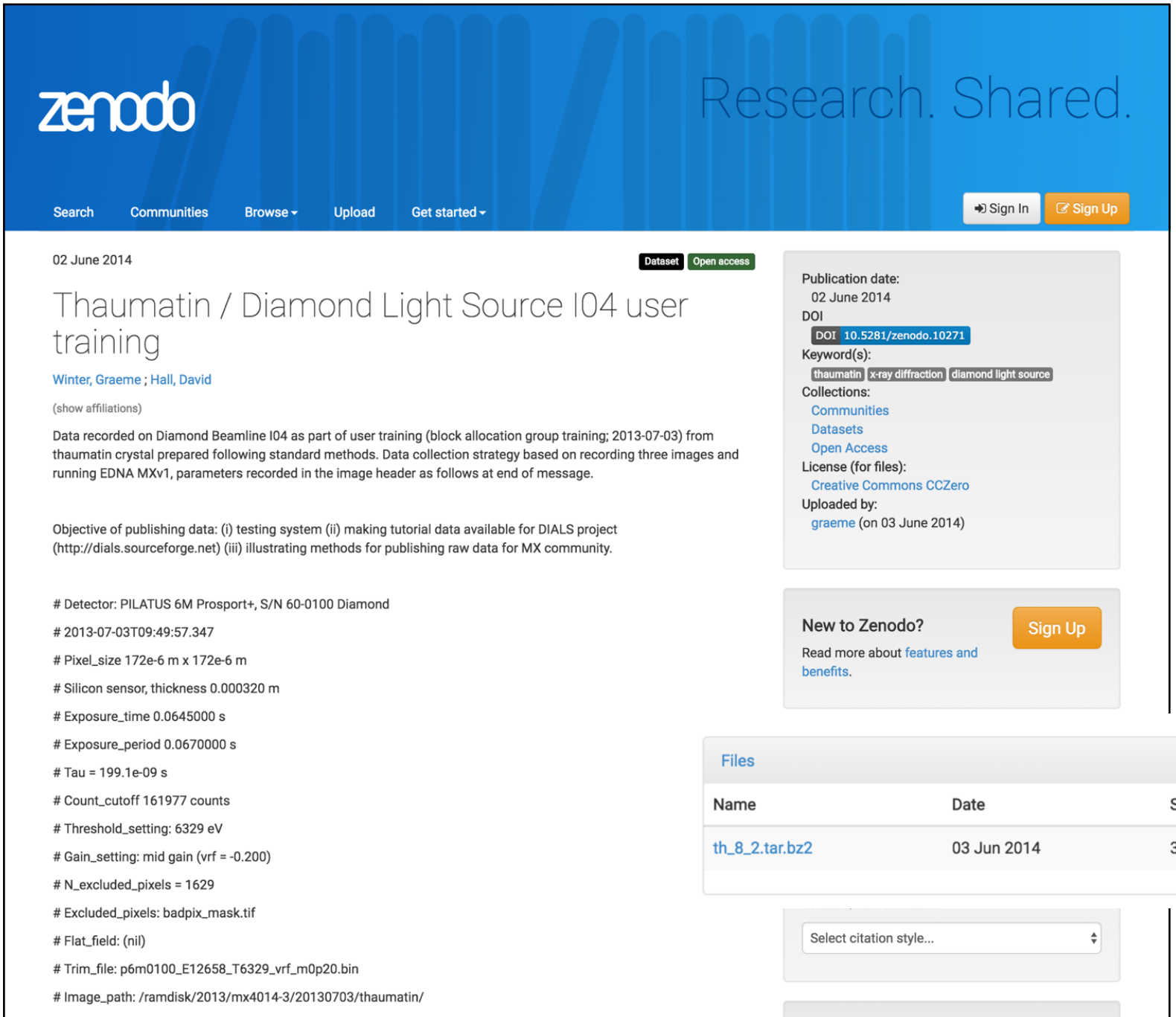
2.1 Coordinate systems and parameters

2.2 Spot prediction

2.3 Standard spot shape

Test data

https://zenodo.org/record/10271#.V6vChZOLRBz



Prepare indexing result

```
mkdir th_8_2
wget https://zenodo.org/record/10271/files/th_8_2.tar.bz2
tar xvf th_8_2.tar.bz2
mkdir xds
cd xds
generate_XDS.INP "../th_8_2_0???.cbf"
vi XDS.INP # Edit SPOT_RANGE= 1 27
           #      JOB= XYCORR INIT COLSPOT IDXREF
xds_par    # Run XDS
```

```
***** REFINED SOLUTION BASED ON INDEXED REFLECTIONS IN SUBTREE # 1 *****

REFINED VALUES OF DIFFRACTION PARAMETERS DERIVED FROM      2988 INDEXED SPOTS
REFINED PARAMETERS:    BEAM ORIENTATION CELL
STANDARD DEVIATION OF SPOT    POSITION (PIXELS)      0.52
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES)     0.19
SPACE GROUP NUMBER      1
UNIT CELL PARAMETERS     57.913    57.829   150.063  89.848  89.989  89.813
REC. CELL PARAMETERS   0.017267  0.017293  0.006664  90.152  90.011  90.187
COORDINATES OF UNIT CELL A-AXIS   -15.071   -53.744   -15.439
COORDINATES OF UNIT CELL B-AXIS    19.947     9.553   -53.433
COORDINATES OF UNIT CELL C-AXIS   135.413   -49.842    41.207
CRYSTAL MOSAICITY (DEGREES)     0.200
LAB COORDINATES OF ROTATION AXIS  1.000000  0.000000  0.000000
DIRECT BEAM COORDINATES (REC. ANGSTROEM)   0.001382  0.000691  1.024327
DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM    1227.43   1194.51
DETECTOR ORIGIN (PIXELS) AT                     1225.35   1193.47
CRYSTAL TO DETECTOR DISTANCE (mm)       265.27
LAB COORDINATES OF DETECTOR X-AXIS  1.000000  0.000000  0.000000
LAB COORDINATES OF DETECTOR Y-AXIS  0.000000  1.000000  0.000000
```

Coordinate systems in XDS

Goniostat system {$\mathbf{m}_1$, $\mathbf{m}_2$, $\mathbf{m}_3$}

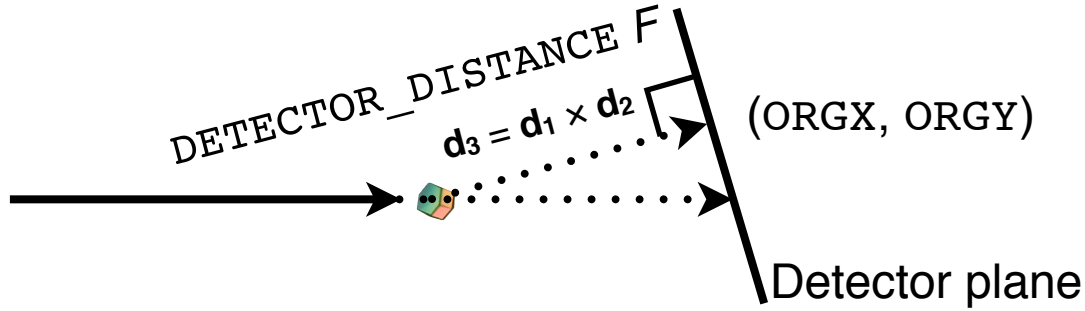
$\mathbf{m}_1 = \mathbf{m}_2 \times \mathbf{S}_0 / | \mathbf{m}_2 \times \mathbf{S}_0 |$

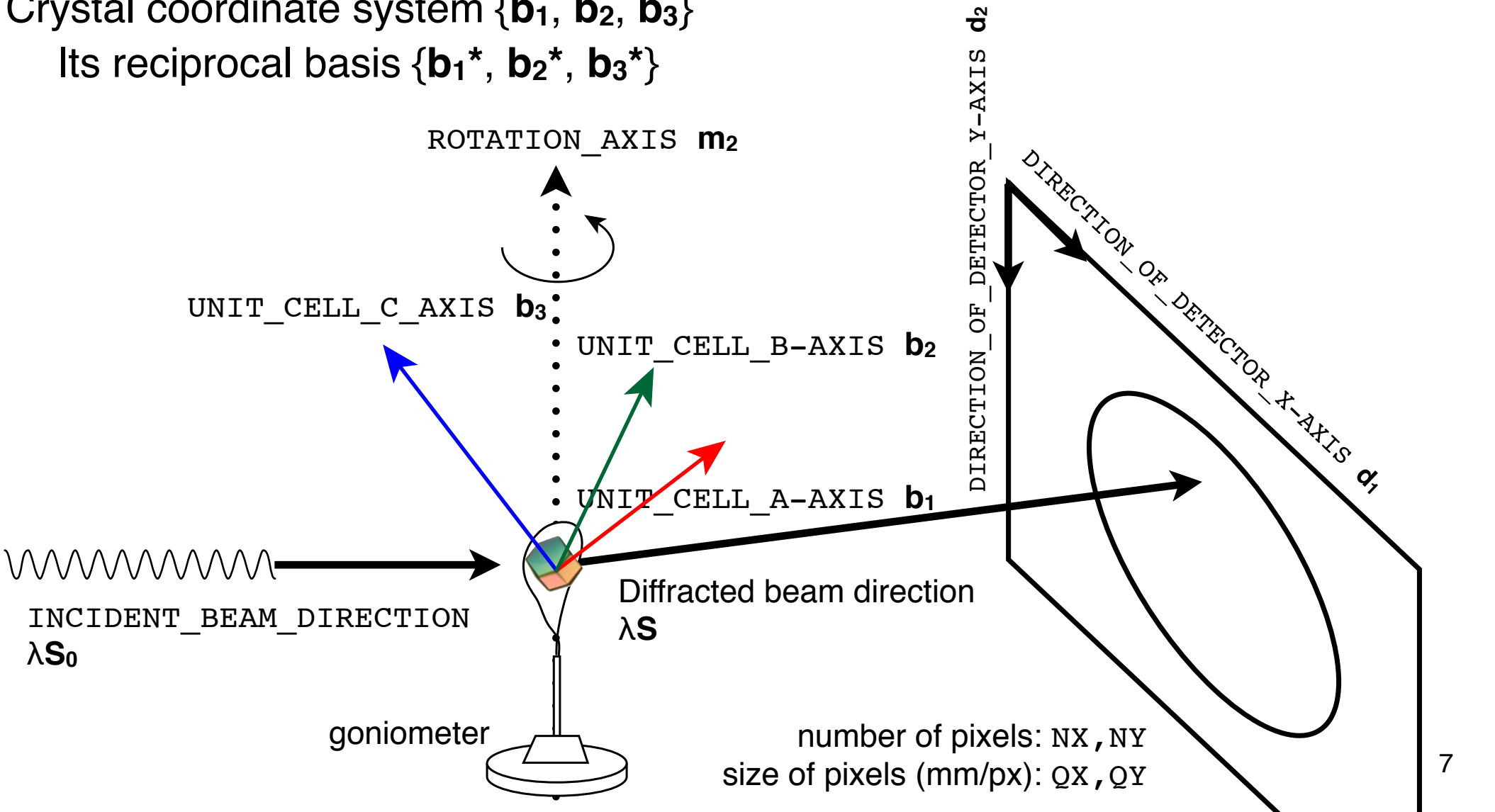
$\mathbf{m}_3 = \mathbf{m}_1 \times \mathbf{m}_2$

Detector system {$\mathbf{d}_1$, $\mathbf{d}_2$, $\mathbf{d}_3$}

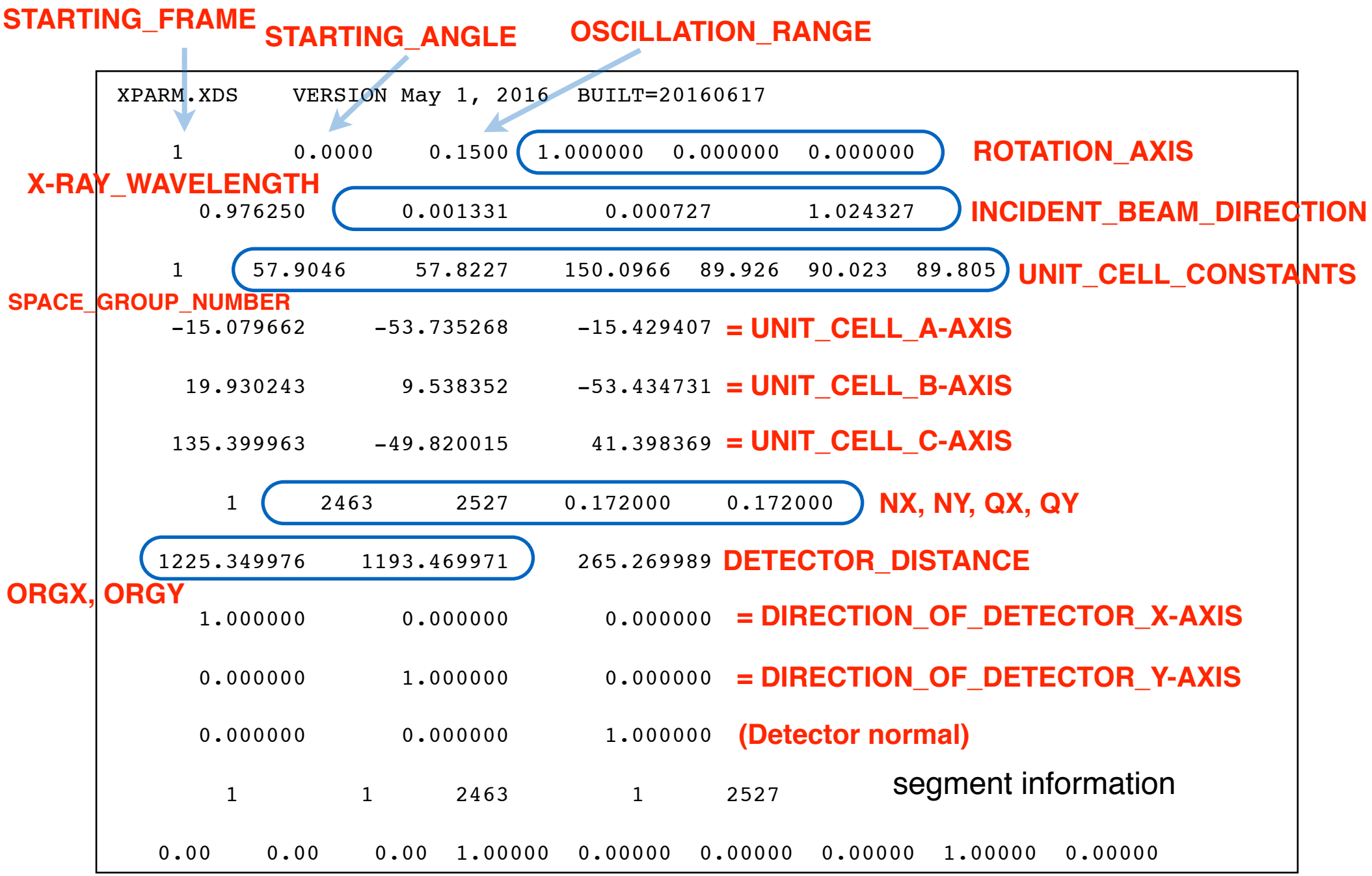
Crystal coordinate system {$\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$}

Its reciprocal basis {$\mathbf{b}_1^*$, $\mathbf{b}_2^*$, $\mathbf{b}_3^*$}



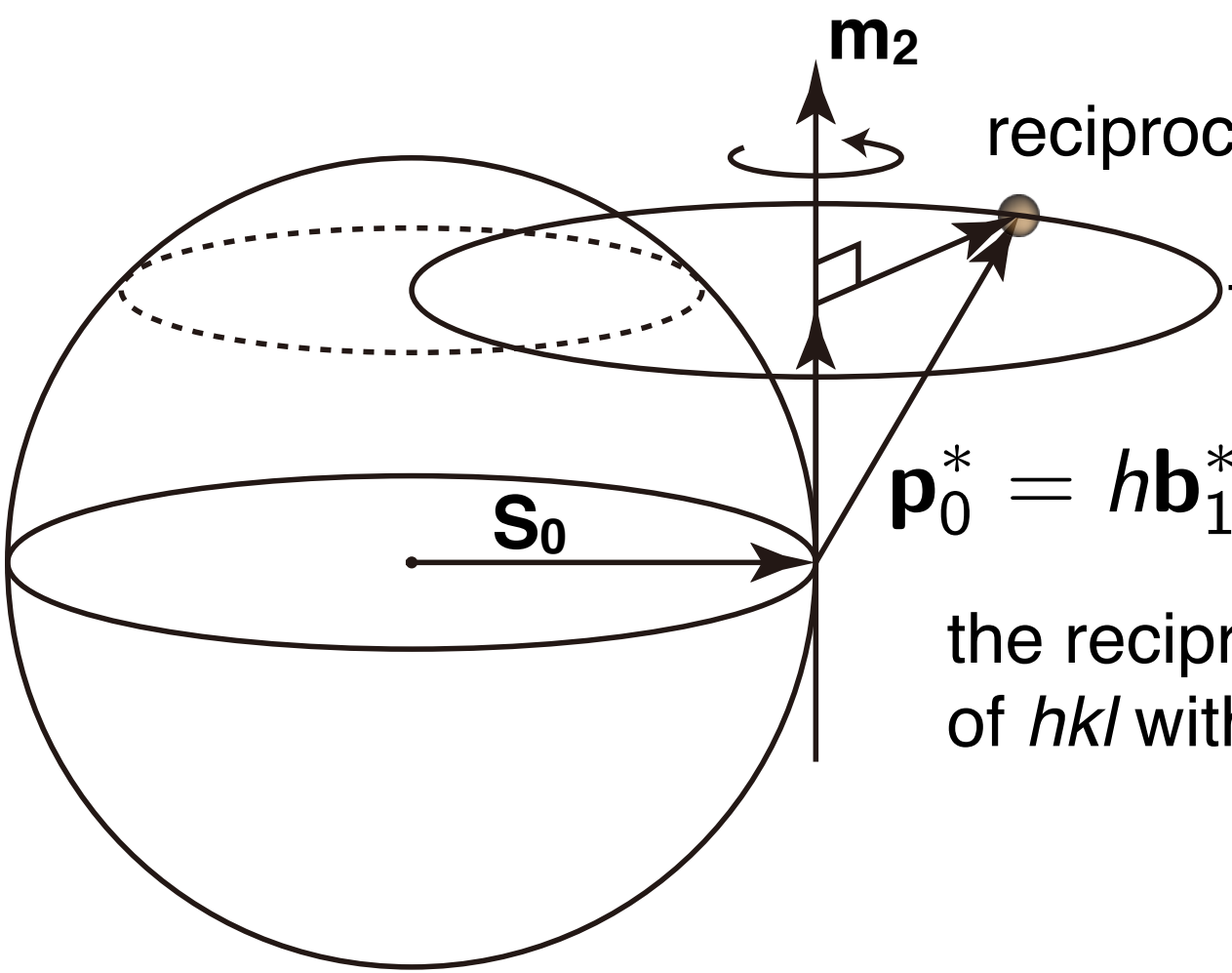


XPARM.XDS


STARTING_FRAME
STARTING_ANGLE
OSCILLATION_RANGE
XPARM.XDS VERSION May 1, 2016 BUILT=20160617
1 0.0000 0.1500 1.000000 0.000000 0.000000
ROTATION_AXIS
X-RAY_WAVELENGTH
0.976250 0.001331 0.000727 1.024327
INCIDENT_BEAM_DIRECTION
1 57.9046 57.8227 150.0966 89.926 90.023 89.805
UNIT_CELL_CONSTANTS
SPACE_GROUP_NUMBER
-15.079662 -53.735268 -15.429407 = UNIT_CELL_A-AXIS
19.930243 9.538352 -53.434731 = UNIT_CELL_B-AXIS
135.399963 -49.820015 41.398369 = UNIT_CELL_C-AXIS
1 2463 2527 0.172000 0.172000
NX, NY, QX, QY
1225.349976 1193.469971 265.269989 DETECTOR_DISTANCE
ORGX, ORGY
1.000000 0.000000 0.000000 = DIRECTION_OF_DETECTOR_X-AXIS
0.000000 1.000000 0.000000 = DIRECTION_OF_DETECTOR_Y-AXIS
0.000000 0.000000 1.000000 (Detector normal)
1 1 2463 1 2527
segment information
0.00 0.00 0.00 1.00000 0.00000 0.00000 0.00000 1.00000 0.00000

How to predict when reflection occurs

At initial state (no rotations)



reciprocal lattice point (rlp)

trajectory of rlp by rotation

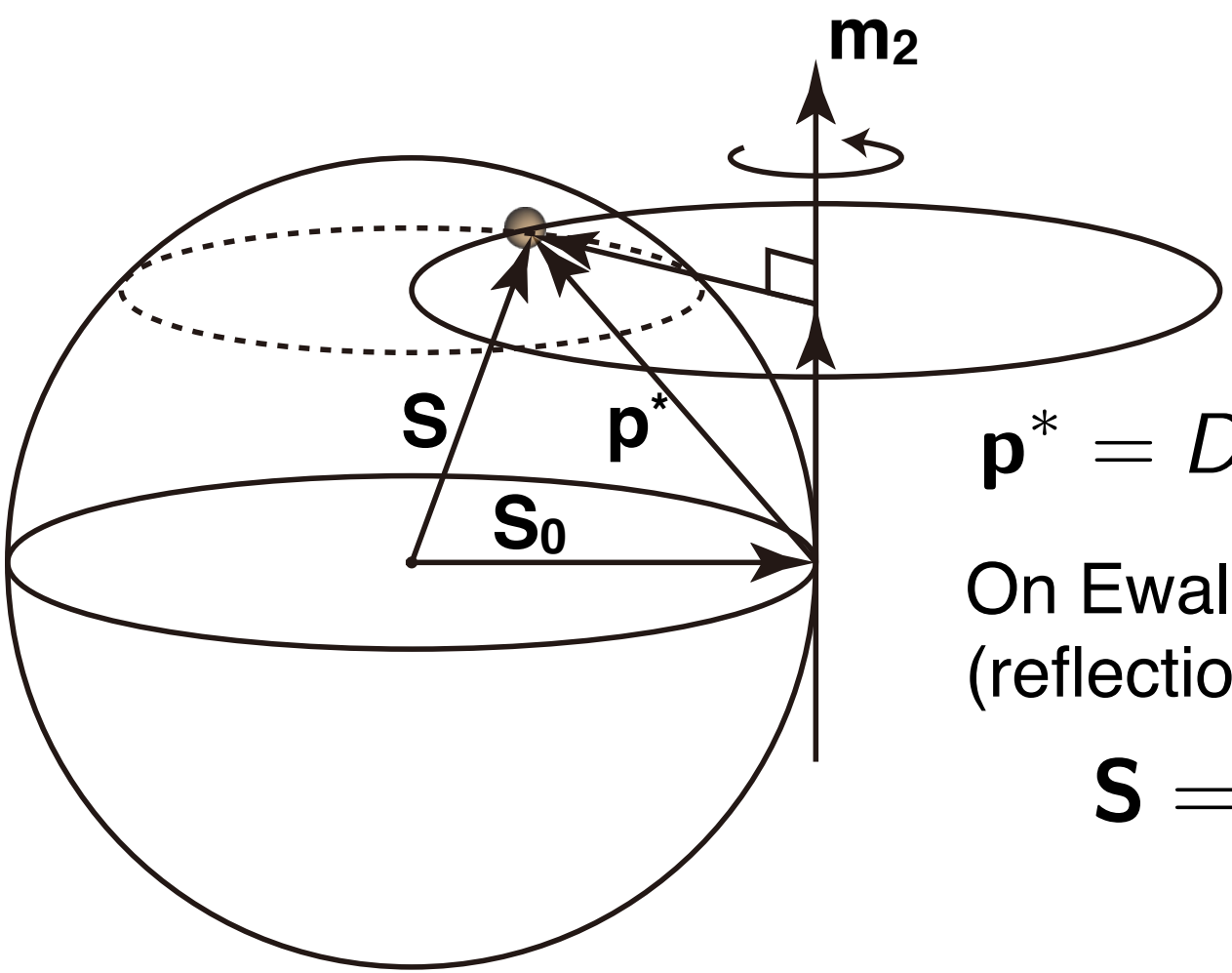
$$\mathbf{p}_0^* = h\mathbf{b}_1^* + k\mathbf{b}_2^* + l\mathbf{b}_3^*$$

the reciprocal space vector
of *hkl* with no rotations

Ewald sphere

How to predict when reflection occurs

After φ rotation



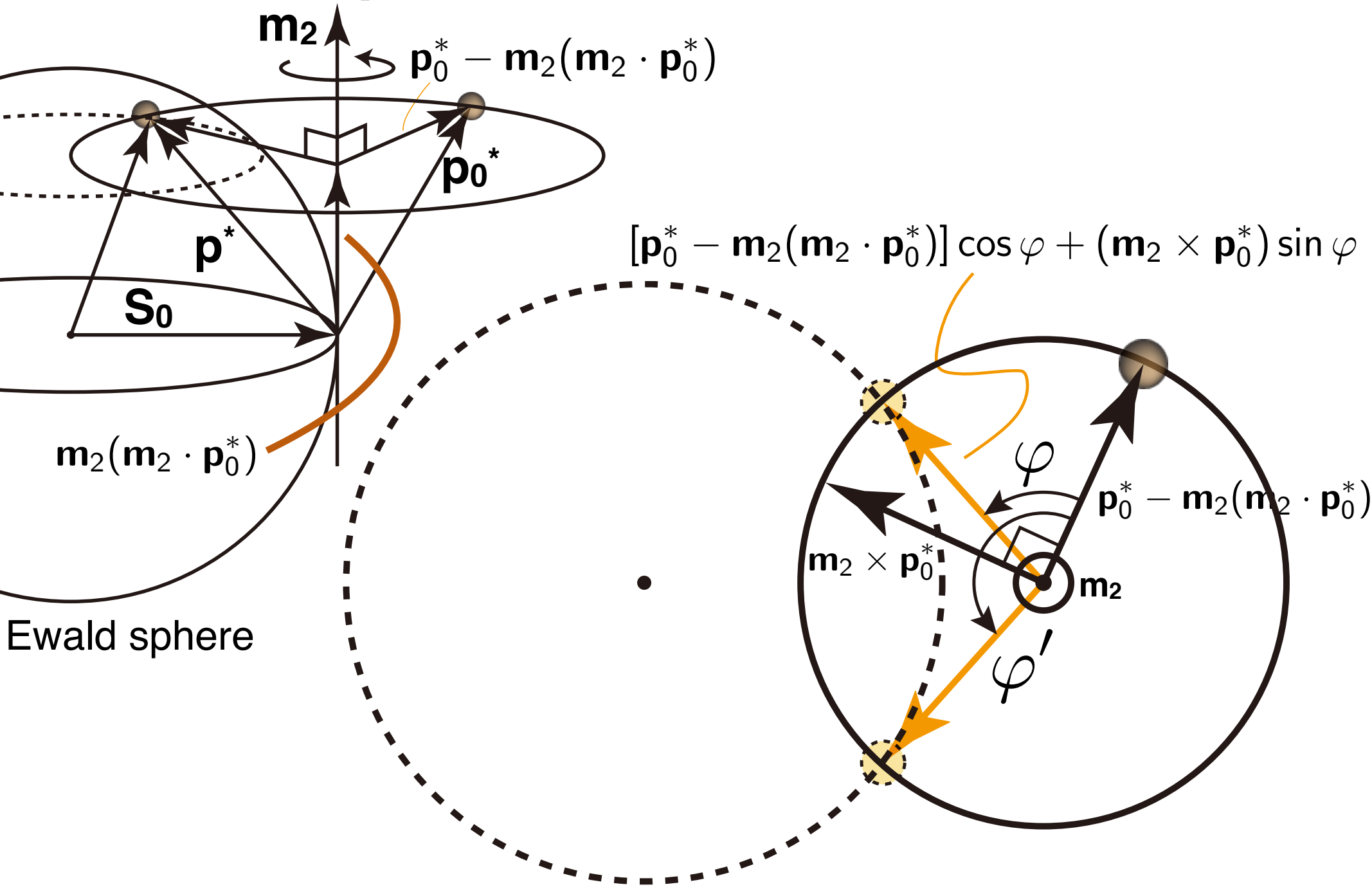
Ewald sphere

$$\mathbf{p}^* = D(\mathbf{m}_2, \varphi)\mathbf{p}_0^*$$

On Ewald sphere
(reflection condition satisfied)

$$\mathbf{S} = \mathbf{S}_0 + \mathbf{p}^*$$

How to predict when reflection occurs



$$\therefore \mathbf{p}^* = \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + [\mathbf{p}_0^* - \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*)]\cos\varphi + (\mathbf{m}_2 \times \mathbf{p}_0^*)\sin\varphi$$

How to predict when reflection occurs

Express $\mathbf{p}_0^*$ with $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$ basis

$$\mathbf{p}_0^* = \mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}_0^*)$$

$$\mathbf{p}^* = \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + [\mathbf{p}_0^* - \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*)]\cos\varphi + (\mathbf{m}_2 \times \mathbf{p}_0^*)\sin\varphi$$

$$\mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}_0^*)$$

$$\mathbf{m}_2 \times \mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_2 \times \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}_0^*) = -\mathbf{m}_3(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_1(\mathbf{m}_3 \cdot \mathbf{p}_0^*)$$

$$= \mathbf{m}_1[(\mathbf{m}_1 \cdot \mathbf{p}_0^*)\cos\varphi + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)\sin\varphi] + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + \mathbf{m}_3[(\mathbf{m}_3 \cdot \mathbf{p}_0^*)\cos\varphi - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)\sin\varphi]$$

$$= \mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}^*) + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}^*) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}^*)$$ expressed with $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$ basis

$$\therefore \begin{cases} (\mathbf{m}_1 \cdot \mathbf{p}_0^*)\cos\varphi + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)\sin\varphi = \mathbf{m}_1 \cdot \mathbf{p}^* \\ (\mathbf{m}_3 \cdot \mathbf{p}_0^*)\cos\varphi - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)\sin\varphi = \mathbf{m}_3 \cdot \mathbf{p}^* \end{cases}$$

$$\iff \begin{cases} \cos\varphi = [(\mathbf{m}_1 \cdot \mathbf{p}_0^*)(\mathbf{m}_1 \cdot \mathbf{p}^*) + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)(\mathbf{m}_3 \cdot \mathbf{p}^*)]/\rho^2 \\ \sin\varphi = [(\mathbf{m}_3 \cdot \mathbf{p}_0^*)(\mathbf{m}_1 \cdot \mathbf{p}^*) - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)(\mathbf{m}_3 \cdot \mathbf{p}^*)]/\rho^2 \end{cases}$$

$$\rho^2 = (\mathbf{m}_1 \cdot \mathbf{p}_0^*)^2 + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)^2 = |\mathbf{p}_0^* - \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*)|^2 = \mathbf{p}_0^{*2} - (\mathbf{m}_2 \cdot \mathbf{p}_0^*)^2$$

(squared distance from $\mathbf{p}_0^*$ to rotation axis)

How to predict when reflection occurs

Express $\mathbf{p}_0^*$ with $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$ basis

$$\mathbf{p}_0^* = \mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}_0^*)$$

$$\mathbf{p}^* = \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + [\mathbf{p}_0^* - \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*)]\cos\varphi + (\mathbf{m}_2 \times \mathbf{p}_0^*)\sin\varphi$$

$$\mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}_0^*)$$

$$\mathbf{m}_2 \times \mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_2 \times \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}_0^*) = -\mathbf{m}_3(\mathbf{m}_1 \cdot \mathbf{p}_0^*) + \mathbf{m}_1(\mathbf{m}_3 \cdot \mathbf{p}_0^*)$$

$$= \mathbf{m}_1[(\mathbf{m}_1 \cdot \mathbf{p}_0^*)\cos\varphi + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)\sin\varphi] + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + \mathbf{m}_3[(\mathbf{m}_3 \cdot \mathbf{p}_0^*)\cos\varphi - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)\sin\varphi]$$

$$= \mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}^*) + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}^*) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}^*)$$ expressed with $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$ basis

$$\therefore \begin{cases} (\mathbf{m}_1 \cdot \mathbf{p}_0^*)\cos\varphi + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)\sin\varphi = \mathbf{m}_1 \cdot \mathbf{p}^* \\ (\mathbf{m}_3 \cdot \mathbf{p}_0^*)\cos\varphi - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)\sin\varphi = \mathbf{m}_3 \cdot \mathbf{p}^* \end{cases}$$ We don't know!

$$\iff \begin{cases} \cos\varphi = [(\mathbf{m}_1 \cdot \mathbf{p}_0^*)(\mathbf{m}_1 \cdot \mathbf{p}^*) + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)(\mathbf{m}_3 \cdot \mathbf{p}^*)]/\rho^2 \\ \sin\varphi = [(\mathbf{m}_3 \cdot \mathbf{p}_0^*)(\mathbf{m}_1 \cdot \mathbf{p}^*) - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)(\mathbf{m}_3 \cdot \mathbf{p}^*)]/\rho^2 \end{cases}$$

$$\rho^2 = (\mathbf{m}_1 \cdot \mathbf{p}_0^*)^2 + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)^2 = |\mathbf{p}_0^* - \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{p}_0^*)|^2 = \mathbf{p}_0^{*2} - (\mathbf{m}_2 \cdot \mathbf{p}_0^*)^2$$

(squared distance from $\mathbf{p}_0^*$ to rotation axis)

How to predict when reflection occurs

When Laue equations satisfied

$$\mathbf{S} = \mathbf{S}_0 + \mathbf{p}^*,\ \mathbf{S}^2 = \mathbf{S}_0^2 \implies \mathbf{p}^{*2} = -2\mathbf{S}_0 \cdot \mathbf{p}^* = \mathbf{p}_0^{*2}$$

Express $\mathbf{S}_0$ and $\mathbf{p}^*$ with $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$ basis

$$-2\Big[\mathbf{m}_1\underbrace{(\mathbf{m}_1 \cdot \mathbf{S}_0)}_{=0} + \mathbf{m}_2(\mathbf{m}_2 \cdot \mathbf{S}_0) + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{S}_0)\Big]\Big[\mathbf{m}_1(\mathbf{m}_1 \cdot \mathbf{p}^*) + \mathbf{m}_2\underbrace{(\mathbf{m}_2 \cdot \mathbf{p}^*)}_{=\mathbf{m}_2 \cdot \mathbf{p}_0^*} + \mathbf{m}_3(\mathbf{m}_3 \cdot \mathbf{p}^*)\Big]$$

$$= -2\Big[(\mathbf{m}_2 \cdot \mathbf{S}_0)(\mathbf{m}_2 \cdot \mathbf{p}_0^*) + (\mathbf{m}_3 \cdot \mathbf{S}_0)(\mathbf{m}_3 \cdot \mathbf{p}^*)\Big] = \mathbf{p}^{*2}$$

as the component along rotation axis does not change by rotation

$$\therefore \mathbf{m}_3 \cdot \mathbf{p}^* = \frac{-\mathbf{p}^{*2}/2 - (\mathbf{m}_2 \cdot \mathbf{S}_0)(\mathbf{m}_2 \cdot \mathbf{p}_0^*)}{\mathbf{m}_3 \cdot \mathbf{S}_0}$$

$$\mathbf{m}_2 \cdot \mathbf{p}^* = \mathbf{m}_2 \cdot \mathbf{p}_0^*$$

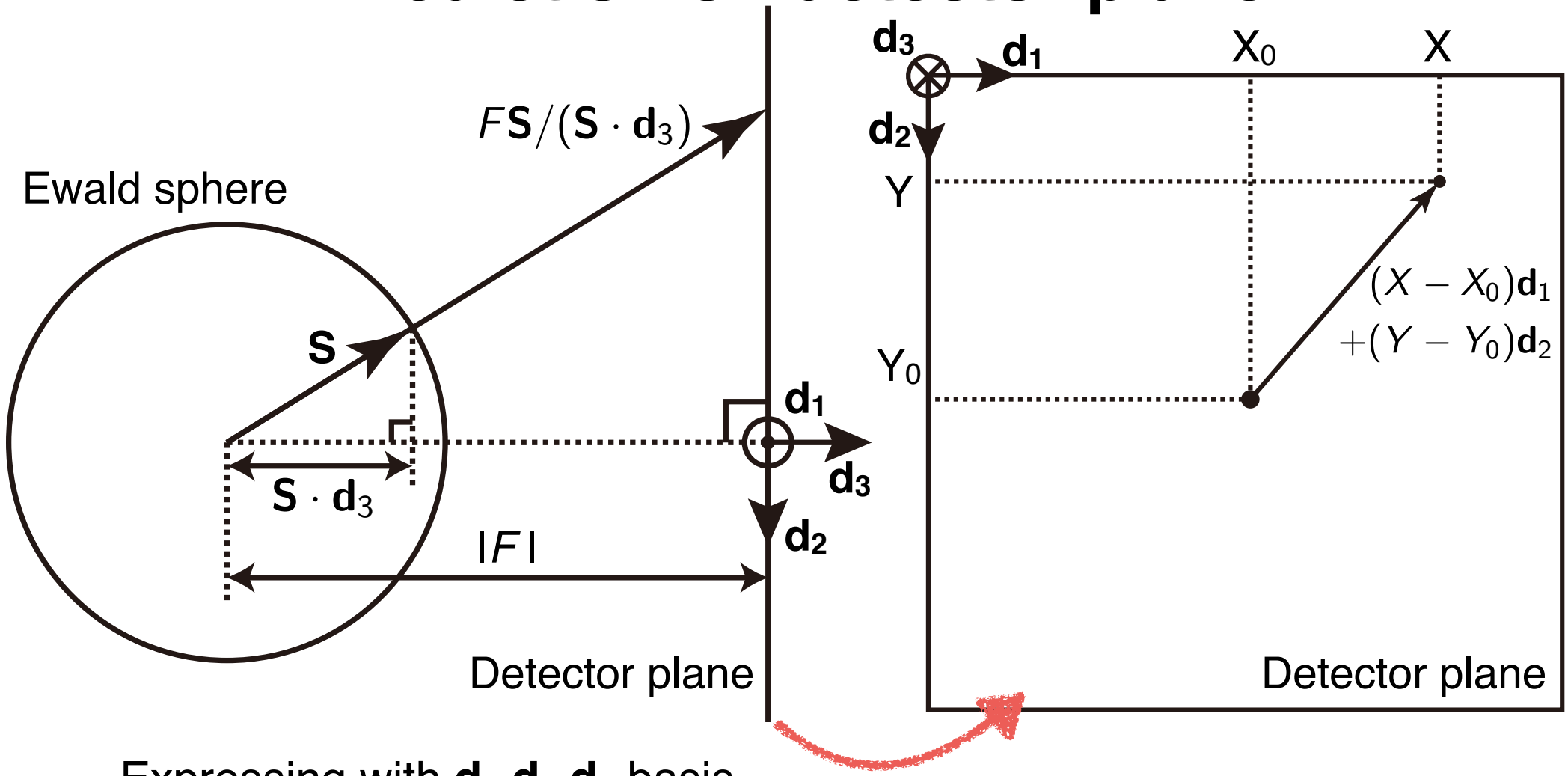
$$\mathbf{m}_1 \cdot \mathbf{p}^* = \pm\sqrt{\mathbf{p}_0^{*2} - (\mathbf{m}_2 \cdot \mathbf{p}^*)^2 - (\mathbf{m}_3 \cdot \mathbf{p}^*)^2}$$ (as $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$ are orthonormal basis)

Finally $\mathbf{p}^*$ has been obtained as components along $\mathbf{m}_1$,$\mathbf{m}_2$,$\mathbf{m}_3$!

But Laue equations have no solutions if $\rho^2 < (\mathbf{m}_3 \cdot \mathbf{p}^*)^2$ or $\mathbf{p}_0^{*2} > 4\mathbf{S}_0^2$

(blind region) (out of limiting sphere)

Prediction on detector plane



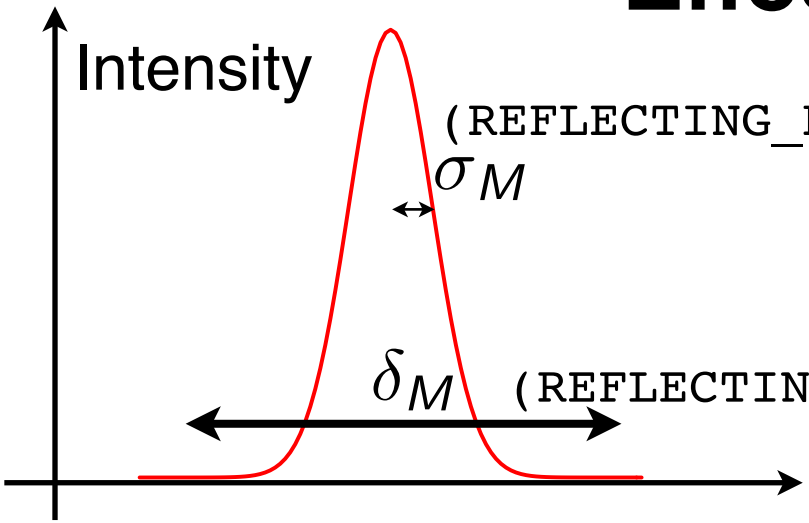
Expressing with $\mathbf{d}_1$,$\mathbf{d}_2$,$\mathbf{d}_3$ basis

$$\begin{aligned} F\mathbf{S}/(\mathbf{S}\cdot\mathbf{d}_3) &= F\mathbf{d}_1(\mathbf{S}\cdot\mathbf{d}_1)/(\mathbf{S}\cdot\mathbf{d}_3) + F\mathbf{d}_2(\mathbf{S}\cdot\mathbf{d}_2)/(\mathbf{S}\cdot\mathbf{d}_3) + F\mathbf{d}_3 \\ &= (X-X_0)\mathbf{d}_1 + (Y-Y_0)\mathbf{d}_2 + F\mathbf{d}_3 \end{aligned}$$

$$\therefore \begin{cases} X = X_0 + F(\mathbf{S}\cdot\mathbf{d}_1)/(\mathbf{S}\cdot\mathbf{d}_3) \\ Y = Y_0 + F(\mathbf{S}\cdot\mathbf{d}_2)/(\mathbf{S}\cdot\mathbf{d}_3) \end{cases}$$

But beam intersects the detector only when $F(\mathbf{S}\cdot\mathbf{d}_3) > 0$

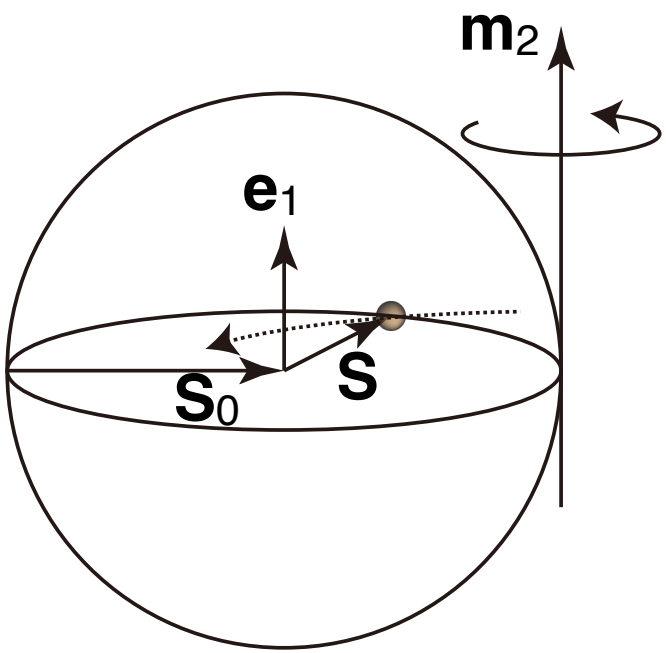
Effect of mosaicity



The standard deviation of Gaussian rocking curve is defined as “mosaicity” in *XDS*

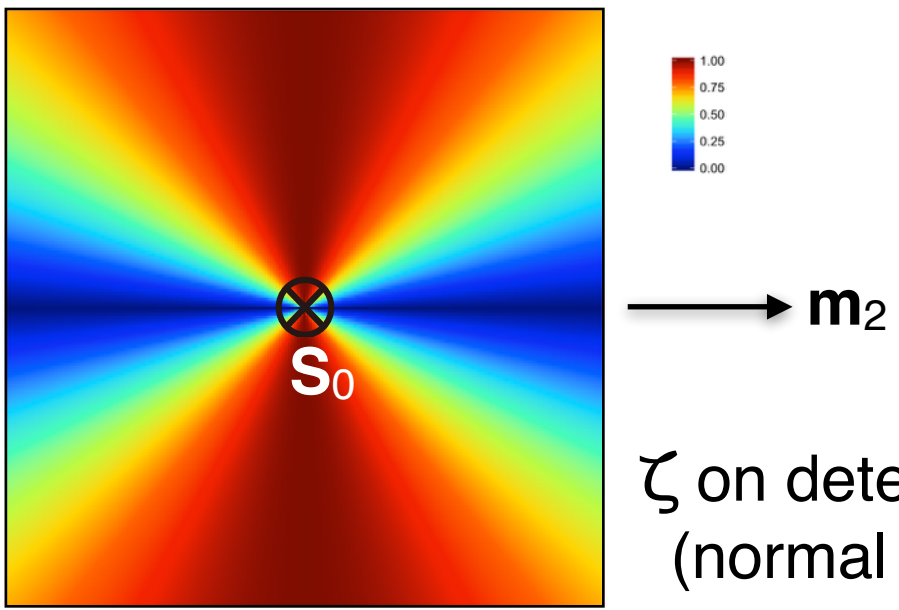
However, the reflecting range is elongated by the factor $1/|\zeta|$

$$\zeta = \mathbf{e}_1 \cdot \mathbf{m}_2 \qquad (\mathbf{e}_1 = \mathbf{S} \times \mathbf{S}_0 / |\mathbf{S} \times \mathbf{S}_0|)$$



Ewald sphere

A reciprocal lattice point crosses the Ewald sphere by the shortest route when $\mathbf{m}_2$ // $\mathbf{e}_1$



ζ on detector plane (normal to beam)

Mathematical summary

Given *hkl*, the reciprocal lattice vector $\mathbf{p}_0^*$ at initial geometry is

$$\mathbf{p}_0^* = h\mathbf{b}_1^* + k\mathbf{b}_2^* + l\mathbf{b}_3^*$$

After φ rotation around $\mathbf{m}_2$ vector, reflection condition is satisfied

$$\mathbf{p}^* = D(\mathbf{m}_2, \varphi)\mathbf{p}_0^*,\ \mathbf{S} = \mathbf{S}_0 + \mathbf{p}^*$$

Here φ can be obtained by

$$\varphi = \tan^{-1} \frac{[(\mathbf{m}_3 \cdot \mathbf{p}_0^*)(\mathbf{m}_1 \cdot \mathbf{p}^*) - (\mathbf{m}_1 \cdot \mathbf{p}_0^*)(\mathbf{m}_3 \cdot \mathbf{p}^*)]/\rho^2}{[(\mathbf{m}_1 \cdot \mathbf{p}_0^*)(\mathbf{m}_1 \cdot \mathbf{p}^*) + (\mathbf{m}_3 \cdot \mathbf{p}_0^*)(\mathbf{m}_3 \cdot \mathbf{p}^*)]/\rho^2}$$

with

$$\begin{cases} \mathbf{m}_3 \cdot \mathbf{p}^* = \frac{-\mathbf{p}^{*2}/2 - (\mathbf{m}_2 \cdot \mathbf{S}_0)(\mathbf{m}_2 \cdot \mathbf{p}_0^*)}{\mathbf{m}_3 \cdot \mathbf{S}_0} \\ \mathbf{m}_2 \cdot \mathbf{p}^* = \mathbf{m}_2 \cdot \mathbf{p}_0^* \\ \mathbf{m}_1 \cdot \mathbf{p}^* = \pm\sqrt{\mathbf{p}_0^{*2} - (\mathbf{m}_2 \cdot \mathbf{p}^*)^2 - (\mathbf{m}_3 \cdot \mathbf{p}^*)^2} \end{cases}$$

Then, the coordinate of the spot on the detector is

$$\begin{cases} X = X_0 + F(\mathbf{S} \cdot \mathbf{d}_1)/(\mathbf{S} \cdot \mathbf{d}_3) \\ Y = Y_0 + F(\mathbf{S} \cdot \mathbf{d}_2)/(\mathbf{S} \cdot \mathbf{d}_3) \end{cases}$$

Standard deviation of the reflecting range is

$$\sigma_M/|\zeta|,\ \zeta = \mathbf{m}_2 \cdot (\mathbf{S} \times \mathbf{S}_0)/|\mathbf{S} \times \mathbf{S}_0|$$

Ready?

Leu us implement a code to calculate the list of (X, Y, φ)

1. Generate a complete set of Miller indices using CCTBX
2. Calculate the list of (X, Y, φ) by matrix calculations using NumPy
3. For a given frame number, generate .adx file which includes (X,Y) coordinates for viewing with Adxv

NumPy

"*Python is fast if you don't use python*"

Pascal (2012) *CCP4BB*
https://www.mail-archive.com/ccp4bb@jiscmail.ac.uk/msg24791.html

- Python is very powerful and easy to use, but slow!
  - For example, to calculate predictions, if we use for-loop for each *hkl*, it would be extremely slow

- NumPy is a free (open-source) package for scientific computing with Python
  - *N*-dimensional array object, linear algebra, FFT, …
  - NumPy data types and functions are implemented in C
  - Very fast if we write the code using NumPy functions

Linear algebra with NumPy

```
In [1]: import numpy
In [2]: a = numpy.array([0.,1.,2.])
In [3]: b = numpy.array([3.,4.,5.])
```

$$a = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}, b = \begin{pmatrix} 3 \\ 4 \\ 5 \end{pmatrix}$$

```
In [4]: b[0]
Out[4]: 3.0
```

Index starts with zero

```
In [5]: a*b
Out[5]: array([  0.,   4.,  10.])
```

$$= \begin{pmatrix} a_0 b_0 \\ a_1 b_1 \\ a_2 b_2 \end{pmatrix}$$

Multiplications of elements

```
In [6]: numpy.dot(a,b)
Out[6]: 14.0
```

$$\sum_i a_i b_i = \mathbf{a} \cdot \mathbf{b}$$

Inner product

```
In [7]: numpy.cross(a,b)
Out[7]: array([-3.,  6., -3.])
```

$$= \mathbf{a} \times \mathbf{b}$$

Cross product

```
In [8]: numpy.linalg.norm(a)
Out[8]: 2.2360679774997898

In [9]: numpy.dot(a, a)
Out[9]: 5.0

In [10]: numpy.sum(a**2)
Out[10]: 5.0
```

$$\mathbf{a} \cdot \mathbf{a} = \sum_i a_i^2 = |\mathbf{a}|^2$$

Linear algebra with NumPy

```
In [11]: A = numpy.array([[0.,1.,2.], [3.,4.,5.], [6.,7.,8.]])
In [12]: A
Out[12]: array([[ 0.,  1.,  2.],
                [ 3.,  4.,  5.],
                [ 6.,  7.,  8.]])
```

$$A = \begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{pmatrix}$$

```
In [13]: A.transpose()
Out[13]: array([[ 0.,  3.,  6.],
                [ 1.,  4.,  7.],
                [ 2.,  5.,  8.]])
```

$$A^t = \begin{pmatrix} 0 & 3 & 6 \\ 1 & 4 & 7 \\ 2 & 5 & 8 \end{pmatrix}$$

```
In [14]: A[1,2]
Out[14]: 5.0

In [15]: A[1,:]
Out[15]: array([ 3.,  4.,  5.])

In [16]: A[:,1]
Out[16]: array([ 1.,  4.,  7.])
```

A[:,1]

$$A = \begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{pmatrix}$$

A[1,:]

```
In [17]: A[1,:] = numpy.array([90, 91, 92])
```

Replace the slice

```
In [18]: A
Out[18]: array([[  0.,   1.,   2.],
                [ 90.,  91.,  92.],
                [  6.,   7.,   8.]])
In [19]: A = numpy.array([[0.,1.,2.], [3.,4.,5.], [6.,7.,8.]])
```

Linear algebra with NumPy

```
In [20]: A*A
Out[20]:
array([[  0.,   1.,   4.],
       [  9.,  16.,  25.],
       [ 36.,  49.,  64.]])
```

Multiplications of elements

```
In [21]: numpy.dot(A, A)
Out[21]:
array([[  15.,   18.,   21.],
       [  42.,   54.,   66.],
       [  69.,   90.,  111.]])
```

Matrix multiplication

```
In [22]: numpy.dot(A, a)
Out[22]: array([  5.,  14.,  23.])
```

$$A\mathbf{a} = \begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}$$

```
In [23]: numpy.dot(a, A)
Out[23]: array([ 15.,  18.,  21.])
```

$$\mathbf{a}^t A = \begin{pmatrix} 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{pmatrix}$$

```
In [24]: numpy.dot(A.transpose(), a)
Out[24]: array([ 15.,  18.,  21.])
```

$$\because (AB)^t = B^t A^t$$

```
In [25]: A.shape
Out[25]: (3, 3)
```

Dimension of array (matrix)

```
In [26]: a.shape
Out[26]: (3,)
```

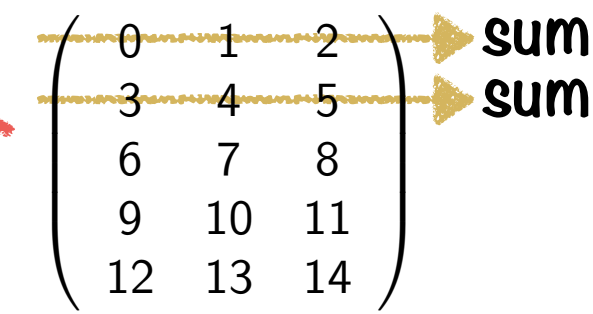
Linear algebra with NumPy

```
In [27]: B = numpy.array(range(15)).reshape(5,3)
In [28]: B
Out[28]:
array([[ 0,  1,  2],
       [ 3,  4,  5],
       [ 6,  7,  8],
       [ 9, 10, 11],
       [12, 13, 14]])
```

$$B = \begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \\ 9 & 10 & 11 \\ 12 & 13 & 14 \end{pmatrix}$$

```
In [29]: numpy.sum(B)
Out[29]: 105
```

sum of all elements




```
In [30]: numpy.sum(B, axis=1)
Out[30]: array([ 3, 12, 21, 30, 39])

In [31]: B_lensq = numpy.sum(B**2, axis=1)

In [32]: B_lensq
Out[32]: array([  5,  50, 149, 302, 509])

In [33]: sel = B_lensq > 100

In [34]: sel
Out[34]: array([False, False,  True,  True,  True], dtype=bool)

In [35]: B[sel]
Out[35]:
array([[ 6,  7,  8],
       [ 9, 10, 11],
       [12, 13, 14]])
```

squared lengths of row-vectors

Take selected rows of B

Linear algebra with NumPy

```
In [36]: d = numpy.array([0,0,1.])
In [37]: C = numpy.cross(B, d)
In [38]: C
Out[38]:
array([[  1.,   0.,   0.],
       [  4.,  -3.,   0.],
       [  7.,  -6.,   0.],
       [ 10.,  -9.,   0.],
       [ 13., -12.,   0.]])

In [39]: numpy.linalg.norm(C, axis=1)
Out[39]: array([  1.        ,   5.        ,   9.21954446,  13.45362405,  17.69180601])

In [40]: C / numpy.linalg.norm(C, axis=1)
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-40-56f89923ab30> in <module>()
----> 1 C / numpy.linalg.norm(C, axis=1)

ValueError: operands could not be broadcast together with shapes (5,3) (5,)

In [41]: C / numpy.linalg.norm(C, axis=1).reshape(C.shape[0], 1)
Out[41]:
array([[ 1.        ,  0.        ,  0.        ],
       [ 0.8       , -0.6       ,  0.        ],
       [ 0.7592566 , -0.65079137,  0.        ],
       [ 0.74329415, -0.66896473,  0.        ],
       [ 0.73480344, -0.6782801 ,  0.        ]])
```

each row = B[i,:] × **d**

each row = B[i,:] × **d** / | B[i,:] × **d** |

How fast?

Test with matrix multiplication: $\begin{pmatrix} h_1 & k_1 & l_1 \\ & \vdots & \\ h_N & k_N & l_N \end{pmatrix} \begin{pmatrix} \mathbf{b}_1^{*t} \\ \mathbf{b}_2^{*t} \\ \mathbf{b}_3^{*t} \end{pmatrix} = \begin{pmatrix} \mathbf{p}_0^{*t} \\ \vdots \\ \vdots \end{pmatrix}$

```
In [1]: import numpy

In [2]: h = numpy.random.randint(-100,100,3*1000000).reshape(1000000,3)

In [3]: a = numpy.array([[-0.00451148, -0.01603847, -0.00454565],
   ...:                  [ 0.00595611,  0.00291487, -0.01597257],
   ...:                  [ 0.00600637, -0.00221528,  0.00184483]])

In [4]: def mul(A, b):
   ...:   ret = numpy.empty(A.shape)
   ...:   for i in xrange(A.shape[0]):
   ...:     for j in xrange(A.shape[1]):
   ...:       ret[i,j] = sum(map(lambda x: x[0]*x[1], zip(A[i,:], b[:,j])))
   ...:   return ret
   ...:

In [5]: %timeit numpy.dot(h, a)
10 loops, best of 3: 23.6 ms per loop

In [6]: %timeit mul(h, a)
1 loops, best of 3: 21.8 s per loop
```

~900× faster
(slow when for-loop was used)

Generate a complete list of miller indices

```
In : from cctbx import crystal
In : from cctbx import miller
In : import numpy
In : xs = crystal.symmetry(unit_cell=(100,100,100,90,90,90),
space_group="p1")
In : miller_set = miller.build_set(xs, anomalous_flag=True, d_min=3.0)
In : miller_set.indices() # flex.miller_index object
Out: <cctbx_array_family_flex_ext.miller_index at 0x10c448050>
In : miller_set.indices()[0]
Out: (-33, -4, 1)
In : miller_set.indices().size() # number of indices
Out: 155330
In : h = numpy.array(miller_set.indices()) # N×3 matrix
In : h
Out: array([[-33,  -4,   1],
            [ 33,   4,  -1],
            [-33,  -4,   2],
            ...,
            [-33,  -4,  -1],
            [ 33,   4,   2],
            [-33,  -4,  -2]])
```

“Main” function of the program

```
if __name__ == "__main__":
    import sys

    xparm_in = sys.argv[1]
    d_min = float(sys.argv[2])
    sigma_m = float(sys.argv[3])
    frames = map(int, sys.argv[4:])

    preds = Predictions()
    print "Reading XPARM.XDS.."
    preds.read_xparm(xparm_in)

    indices = preds.prep_indices(d_min)

    print "Calculating the predicted centroids.."
    preds.calc_centroids(indices)

    for frame in frames:
        print "Calculating the predictions on frame %d.." % frame
        pindices, pdata = preds.get_predicted_positions(sigma_m, frame)

        ofs = open("prediction_%.6d.adx" % frame, "w")
        for (h,k,l), (x, y, phi, zeta) in zip(pindices, pdata):
            ofs.write("%d %d %d %d %d\n"%(x,y, h,k,l))

        ofs.close()
```

Parsing XPARM.XDS

```
XPARM.XDS    VERSION May 1, 2016  BUILT=20160617
    1        0.0000    0.1500  1.000000  0.000000  0.000000
      0.976250       0.001331       0.000727       1.024327
    1     57.9046     57.8227    150.0966  89.926  90.023  89.805
   -15.079662     -53.735268     -15.429407
    19.930243       9.538352     -53.434731
   135.399963     -49.820015      41.398369
       1      2463      2527    0.172000    0.172000
  1225.349976    1193.469971     265.269989
     1.000000       0.000000       0.000000
     0.000000       1.000000       0.000000
     0.000000       0.000000       1.000000
       1         1      2463         1      2527
  0.00    0.00    0.00  1.00000  0.00000  0.00000  0.00000  1.00000  0.00000
```

```
def read_xparm(self, xpin):
    fin = open(xpin)
    assert "XPARM.XDS" in fin.readline()

    # Line 2
    sp = fin.readline().split()
    self.starting_frame = int(sp[0])
    self.starting_angle, self.osc_range = float(sp[1]), float(sp[2])
    m2 = numpy.array(map(float, sp[3:6]))

    # Line 3
    sp = fin.readline().split()
    self.wavelength = float(sp[0])
    incident_beam = numpy.array(map(float, sp[1:4]))
    self.s0 = incident_beam / numpy.linalg.norm(incident_beam) / self.wavelength

    m = numpy.empty(dtype=numpy.float, shape=(3,3))
    m[:,1] = m2 / numpy.linalg.norm(m2)
    m[:,0] = numpy.cross(m[:,1], self.s0)
    m[:,0] /= numpy.linalg.norm(m[:,0])
    m[:,2] = numpy.cross(m[:,0], m[:,1])
    self.m_matrix = m
```

$\mathbf{m}_2$

$$|\mathbf{S}_0| = 1/\lambda$$

$$\begin{pmatrix} \mathbf{m}_1 & \mathbf{m}_2 & \mathbf{m}_3 \end{pmatrix} = \begin{pmatrix} \frac{\mathbf{m}_2 \times \mathbf{S}_0}{|\mathbf{m}_2 \times \mathbf{S}_0|} & \mathbf{m}_2 & \mathbf{m}_1 \times \mathbf{m}_2 \end{pmatrix}$$

Parsing XPARM.XDS

```
XPARM.XDS    VERSION May 1, 2016  BUILT=20160617
     1        0.0000    0.1500  1.000000  0.000000  0.000000
       0.976250       0.001331       0.000727       1.024327
     1     57.9046     57.8227    150.0966  89.926  90.023  89.805
    -15.079662     -53.735268     -15.429407
     19.930243       9.538352     -53.434731
    135.399963     -49.820015      41.398369
        1      2463      2527    0.172000    0.172000
  1225.349976    1193.469971     265.269989
     1.000000       0.000000       0.000000
     0.000000       1.000000       0.000000
     0.000000       0.000000       1.000000
        1         1      2463         1      2527
  0.00    0.00    0.00  1.00000  0.00000  0.00000  0.00000  1.00000  0.00000
```

```
# Line 4
sp = fin.readline().split()
self.crystal_symmetry = crystal.symmetry(unit_cell=map(float, sp[1:7]),
                                         space_group_symbol=int(sp[0]))


# Line 5,6,7 real space vectors
a_axis = map(float, fin.readline().split())
b_axis = map(float, fin.readline().split())
c_axis = map(float, fin.readline().split())

b_mat = numpy.array([a_axis, b_axis, c_axis]).transpose()
self.astar_matrix = numpy.linalg.inv(b_mat)

# Line 8 detector dimensions and pixel size
sp = fin.readline().split()
self.nxy = map(int, sp[1:3]) # NX, NY
self.qxy = map(float, sp[3:5]) # QX, QY
```

$$\begin{pmatrix} \mathbf{b}_1^{*t} \\ \mathbf{b}_2^{*t} \\ \mathbf{b}_3^{*t} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \mathbf{b}_3 \end{pmatrix}^{-1}$$

Parsing XPARM.XDS

```
XPARM.XDS    VERSION May 1, 2016  BUILT=20160617
    1        0.0000    0.1500  1.000000  0.000000  0.000000
      0.976250       0.001331       0.000727       1.024327
    1     57.9046     57.8227    150.0966  89.926  90.023  89.805
    -15.079662     -53.735268     -15.429407
     19.930243       9.538352     -53.434731
    135.399963     -49.820015      41.398369
        1      2463      2527    0.172000    0.172000
   1225.349976    1193.469971     265.269989
      1.000000       0.000000       0.000000
      0.000000       1.000000       0.000000
      0.000000       0.000000       1.000000
        1         1      2463         1      2527
   0.00    0.00    0.00  1.00000  0.00000  0.00000  0.00000  1.00000  0.00000
```

```
# Line 9 ORGX,Y & detector distance
sp = fin.readline().split()
self.orgxy = map(float, sp[:2])
self.detector_F = float(sp[2])

# Line 10,11,12
d1 = map(float, fin.readline().split())
d2 = map(float, fin.readline().split())
d3 = map(float, fin.readline().split())

self.d_matrix = numpy.array([d1,d2,d3]).transpose()
```

$$\begin{pmatrix} \mathbf{d}_1 & \mathbf{d}_2 & \mathbf{d}_3 \end{pmatrix}$$

Implementation of centroid calculation

```
def calc_centroids(self, indices):
    h = numpy.array(indices) # hkl in each row
    m, d, a, F = self.m_matrix, self.d_matrix, self.astar_matrix, self.detector_F
    x0, y0 = self.orgxy
    qx, qy = self.qxy
    s0 = self.s0

    p0s = numpy.dot(h, a)
    p0s_m = numpy.dot(p0s, m)

    s0_m = numpy.dot(m.transpose(), s0)

    p0s_lensq = numpy.sum(p0s**2, axis=1)
```

$$\begin{pmatrix} h_1 & k_1 & l_1 \\ & \vdots & \\ h_N & k_N & l_N \end{pmatrix} \begin{pmatrix} \mathbf{b}_1^{*t} \\ \mathbf{b}_2^{*t} \\ \mathbf{b}_3^{*t} \end{pmatrix} = \begin{pmatrix} \mathbf{p}_0^{*t} \\ \vdots \\ \vdots \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{p}_0^{*t} \\ \vdots \end{pmatrix} \begin{pmatrix} \mathbf{m}_1 & \mathbf{m}_2 & \mathbf{m}_3 \end{pmatrix} = \begin{pmatrix} (\mathbf{m}_1 \cdot \mathbf{p}_0^*) & (\mathbf{m}_2 \cdot \mathbf{p}_0^*) & (\mathbf{m}_3 \cdot \mathbf{p}_0^*) \\ & \vdots & \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{m}_1{}^t \\ \mathbf{m}_2{}^t \\ \mathbf{m}_3{}^t \end{pmatrix} \cdot \mathbf{S}_0 = \begin{pmatrix} \mathbf{m}_1 \cdot \mathbf{S}_0 \\ \mathbf{m}_2 \cdot \mathbf{S}_0 \\ \mathbf{m}_3 \cdot \mathbf{S}_0 \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{p}_0^{*2} \\ \vdots \end{pmatrix}$$

Implementation of centroid calculation

$$\begin{pmatrix} (\mathbf{m}_1 \cdot \mathbf{p}^*) & (\mathbf{m}_2 \cdot \mathbf{p}^*) & (\mathbf{m}_3 \cdot \mathbf{p}^*) \\ & \vdots & \end{pmatrix}$$

$$\begin{cases} \mathbf{m}_3 \cdot \mathbf{p}^* = \dfrac{-\mathbf{p}^{*2}/2 - (\mathbf{m}_2 \cdot \mathbf{S}_0)(\mathbf{m}_2 \cdot \mathbf{p}_0^*)}{\mathbf{m}_3 \cdot \mathbf{S}_0} \\ \mathbf{m}_2 \cdot \mathbf{p}^* = \mathbf{m}_2 \cdot \mathbf{p}_0^* \\ \mathbf{m}_1 \cdot \mathbf{p}^* = \pm\sqrt{\mathbf{p}_0^{*2} - (\mathbf{m}_2 \cdot \mathbf{p}^*)^2 - (\mathbf{m}_3 \cdot \mathbf{p}^*)^2} \end{cases}$$

```
ps_m = numpy.empty(p0s_m.shape)
ps_m[:,2] = (-0.5*p0s_lensq - s0_m[1]*p0s_m[:,1]) / s0_m[2]
ps_m[:,1] = p0s_m[:,1]
ps_m[:,0] = p0s_lensq - ps_m[:,1]**2 - ps_m[:,2]**2 # sqrt after check

sel_ok = ps_m[:,0] > 0 # No solution (blind region) if < 0
h, p0s_m, ps_m = h[sel_ok], p0s_m[sel_ok], ps_m[sel_ok]
ps_m[:,0] = numpy.sqrt(ps_m[:,0])

self.predicted_hkl = numpy.empty((0, 3), dtype=numpy.int) # h,k,l
self.predicted_data = numpy.empty((0, 4)) # x, y, phi, zeta
```

Implementation of centroid calculation

```
for p1sign in (+1, -1):
    ps_m[:,0] *= p1sign
    phi = numpy.arctan2(p0s_m[:,2]*ps_m[:,0]-p0s_m[:,0]*ps_m[:,2],
                        p0s_m[:,0]*ps_m[:,0]+p0s_m[:,2]*ps_m[:,2])
    e1_m = numpy.cross(ps_m, s0_m)
    e1_m /= numpy.linalg.norm(e1_m, axis=1).reshape(e1_m.shape[0], 1)
    zeta = e1_m[:,1]
    s = s0 + numpy.dot(ps_m, m.transpose())
    s_d = numpy.dot(s, d)
    sel_ok = F*s_d[:,2] > 0
    s_d, h_ok, phi, zeta = s_d[sel_ok], h[sel_ok], phi[sel_ok], zeta[sel_ok]

    xdet = x0 + F*s_d[:,0]/s_d[:,2]/qx
    ydet = y0 + F*s_d[:,1]/s_d[:,2]/qy

    self.predicted_hkl = numpy.row_stack([self.predicted_hkl, h_ok])
    self.predicted_data = numpy.row_stack([self.predicted_data,
                                           numpy.column_stack([xdet, ydet, phi, zeta])])
```

$$\varphi = \tan^{-1}\frac{\rho^2 \sin\varphi}{\rho^2 \cos\varphi}$$

$$\begin{pmatrix} (\mathbf{m}_1 \cdot \mathbf{e}_1) & (\mathbf{m}_2 \cdot \mathbf{e}_2) & (\mathbf{m}_3 \cdot \mathbf{e}_3) \\ & \vdots & \end{pmatrix} = \zeta$$

$$\begin{pmatrix} (\mathbf{d}_1 \cdot \mathbf{S}) & (\mathbf{d}_2 \cdot \mathbf{S}) & (\mathbf{d}_3 \cdot \mathbf{S}) \\ & \vdots & \end{pmatrix}$$

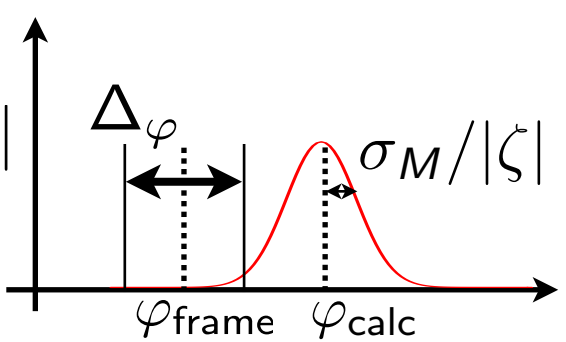
$$\begin{cases} X = X_0 + F(\mathbf{S} \cdot \mathbf{d}_1)/(\mathbf{S} \cdot \mathbf{d}_3) \\ Y = Y_0 + F(\mathbf{S} \cdot \mathbf{d}_2)/(\mathbf{S} \cdot \mathbf{d}_3) \end{cases}$$

Select predictions on specific frame

```
def get_predicted_positions(self, sigma_m, frame, esd_factor=3):
    phi = self.starting_angle + self.osc_range*(frame-self.starting_frame+0.5)
    print "  Phi at frame %d = %.3f" % (frame, phi)

    phi, sigma_m, osc_range = numpy.deg2rad([phi, sigma_m, self.osc_range])

    phi_calc = self.predicted_data[:,2]
    zeta = self.predicted_data[:,3]

    phi_diff = numpy.fmod(phi_calc - phi, 2.*numpy.pi)
    phi_diff[phi_diff < -numpy.pi] += 2.*numpy.pi
    phi_diff[phi_diff > numpy.pi] -= 2.*numpy.pi

    sel = numpy.abs(phi_diff) < osc_range/2. + esd_factor*sigma_m/numpy.abs(zeta)
    return self.predicted_hkl[sel], self.predicted_data[sel]
```

Make the difference in [-π, π] range

Predict if $|\varphi_{calc} - \varphi_{frame}| < \Delta_\varphi/2 + 3\sigma_M/|\zeta|$

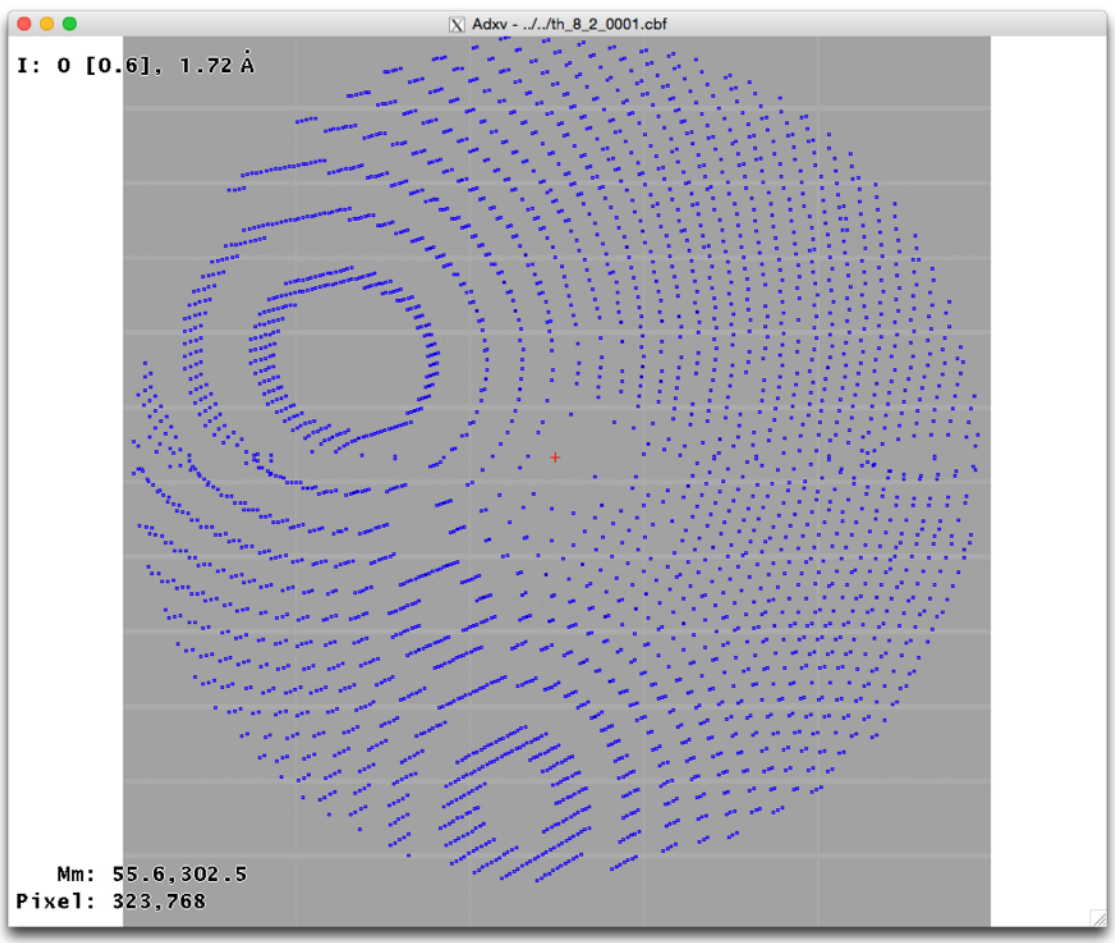


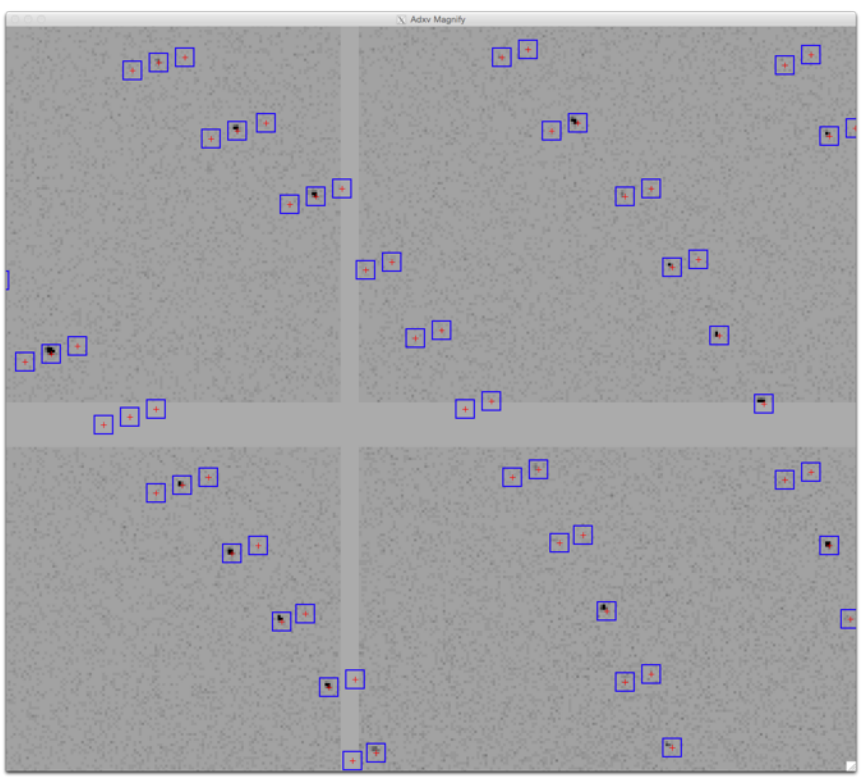
Result

```
$ phenix.python ./prediction.py ./XPARM.XDS 1.5 0.06928 1
```

```
Reading XPARM.XDS..
Calculating the predicted centroids..
Calculating the predictions on frame 1..
  Phi at frame 1 = 0.075
```

```
$ adxv ../th_8_2_0001.cbf prediction_000001.adx
```



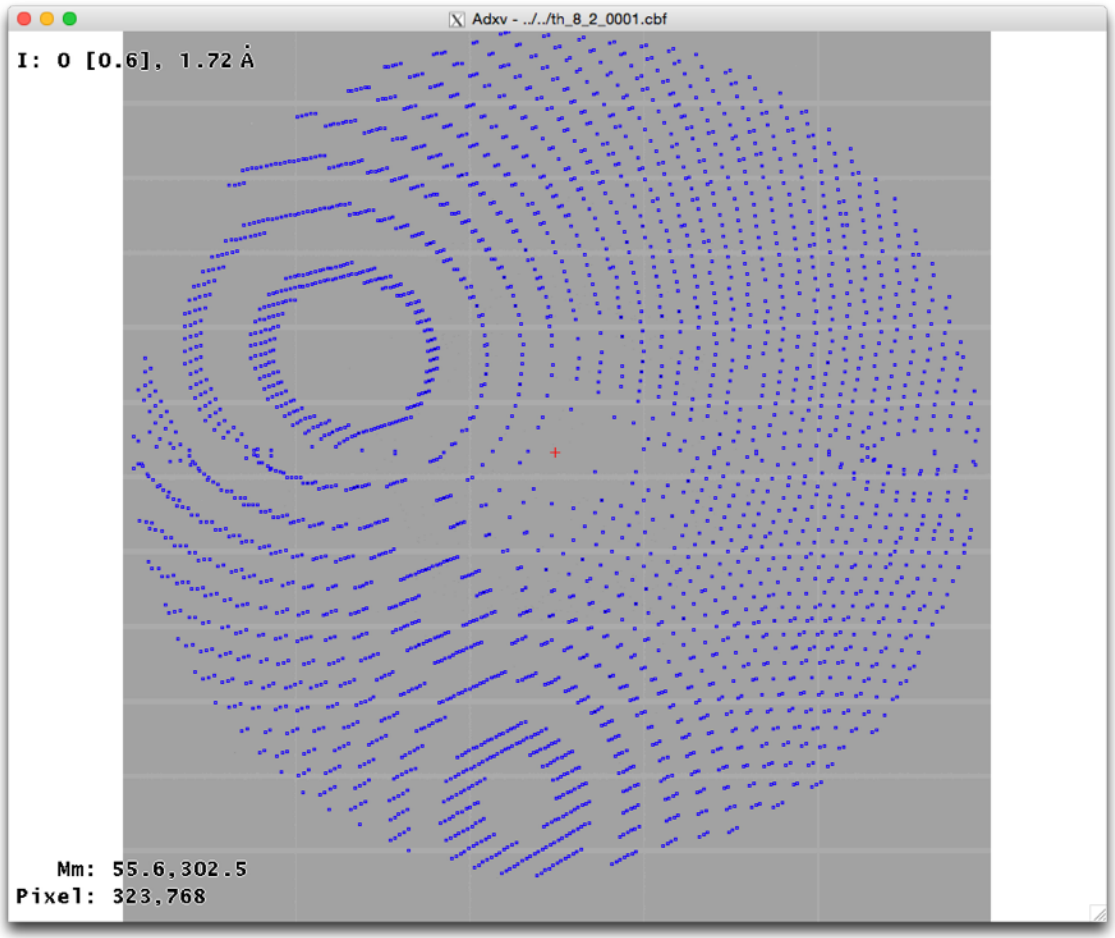


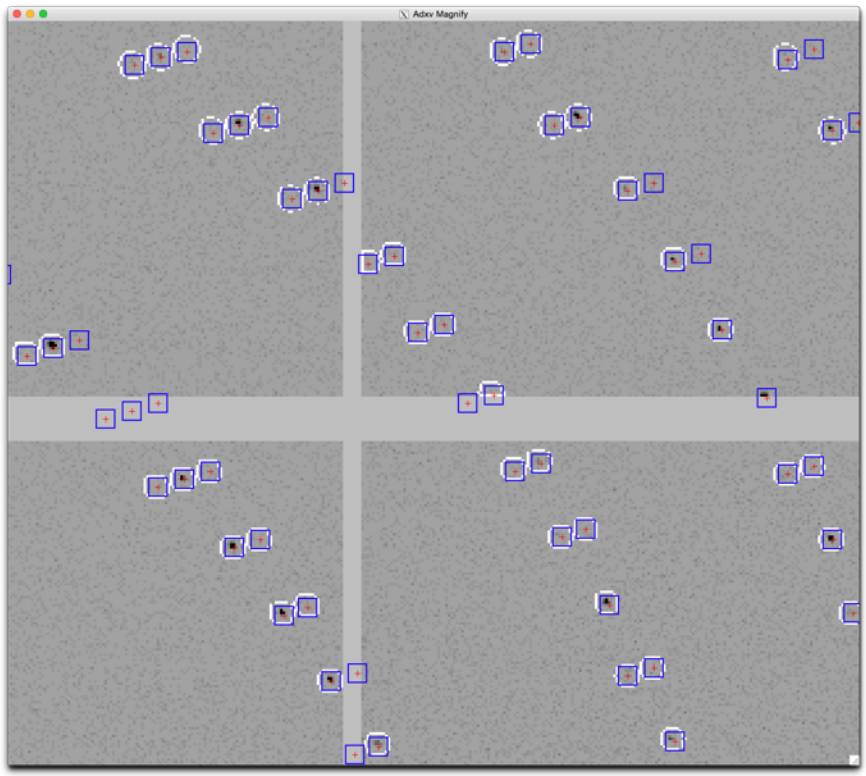
Result

```
$ phenix.python ./prediction.py ./XPARM.XDS 1.5 0.06928 1
```

```
Reading XPARM.XDS..
Calculating the predicted centroids..
Calculating the predictions on frame 1..
  Phi at frame 1 = 0.075
```

```
$ adxv ../th_8_2_0001.cbf prediction_000001.adx
```





Final remarks

- We wrote a Python code to calculate reflection centroids and make a prediction on specific frames

- There are relatively large errors in “Lorentz zone”
  - We only calculated (x,y,φ) of the centroids of reflections
  - To know more accurate spot positions on a frame, we may need to model individual reflection routes as *XDS* ver. Dec 31, 2011 (and newer) does

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* http://d.hatena.ne.jp/biochem_fan/20150727/1437982461

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