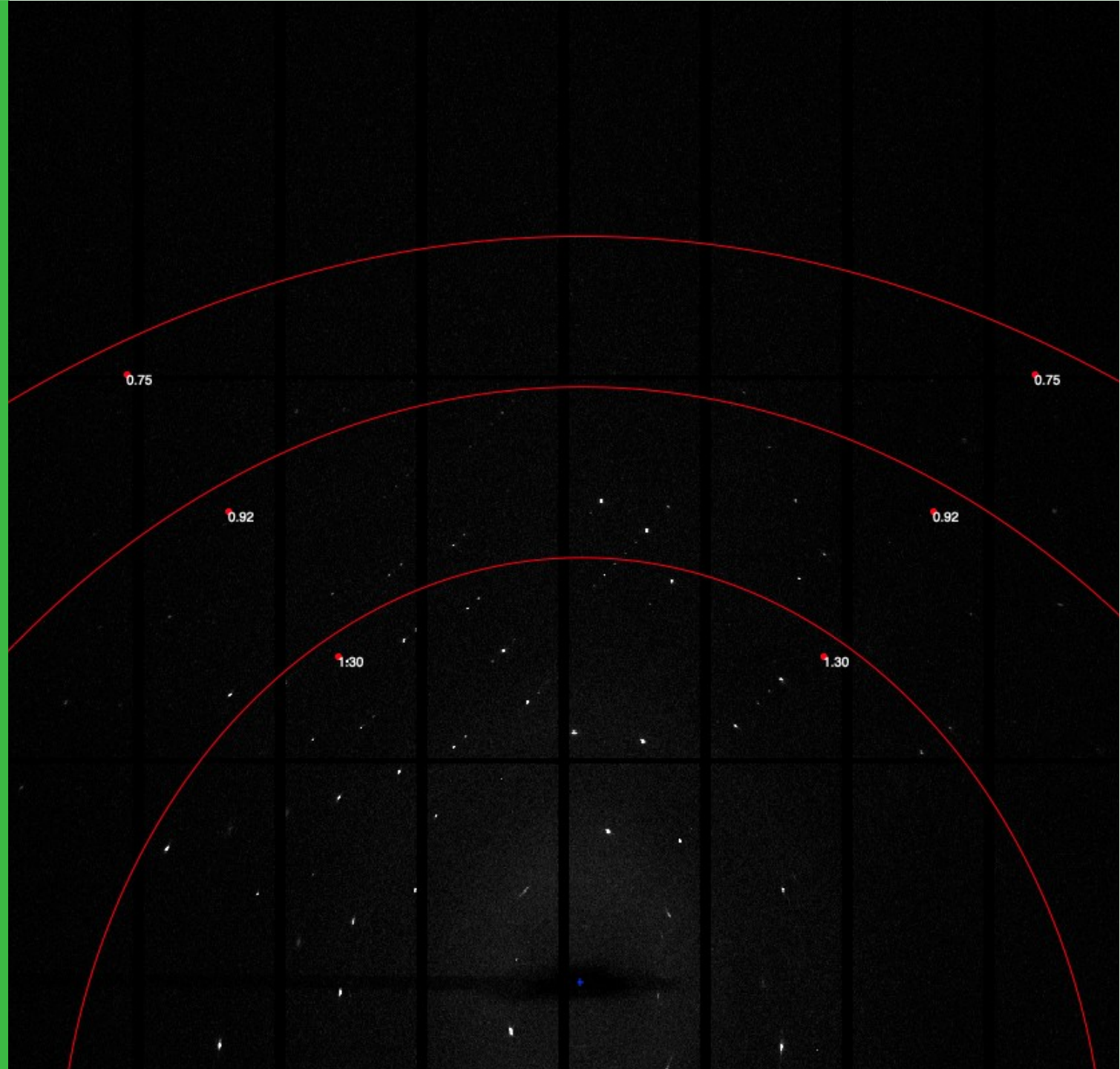


Gold Standard NXmx @ DLS

**HDRMX virtual
workshop
August 2020**

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for Graeme Winter**



NXmx at DLS

Diamond unusual ? — Points of Difference

- both Producer and Consumer — GDA / xia2 & DIALS
- biological and chemical crystallography
- use NeXus extensively outside of MX and beyond Eiger detectors
- write all our own files — GDA makes NeXus / master* files and ODIN captures the data to HDF5

* name under review

Producer

- already extensively using full imgCIF / CBF to describe experiment geometry including e.g. 2θ axis
- want to be able to record experiment metadata correctly — but easily too
- existing standard fine for one-run-per-set and “standard” geometry
- dependency chain great — if and only if you get it right
- can cope with more complex collections if you use Virtual Data Sets (VDS)

Complex data sets

**Going beyond one scan / one data set / one file
sequence**

VDS

- Virtual Data Set — allows mapping between bytes on disk and logical view of the data
- offers potential for a number of sophisticated use cases
For example: inverse beam experiments, multi-trigger data sets
- requires use of HDF5 libraries to read correctly
(i.e. Neggia won't work but Durin will)

Inverse beam

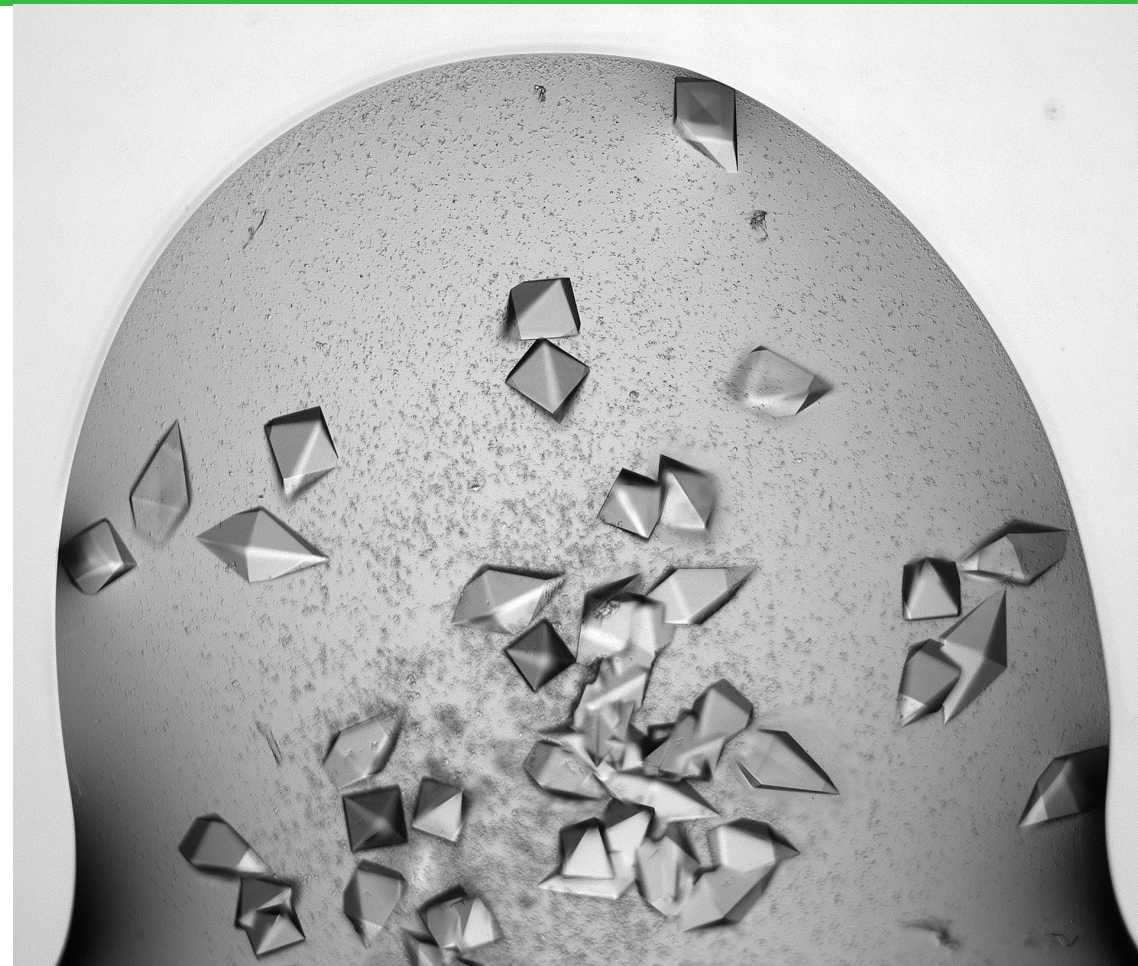
Example: Arm once, use 36 triggers, each trigger for 10° of data
0– 10° , 180– 190° , 10– 20° , 190– 200° , ...

```
master A-----+-----...----+
      |           |           |
      v           v           v
    [A0][B0][A1][B1]...[A17][B17]
          ^         ^         ^
          |         |         |
master B --+-----+-----...----+
```

- data captured as continuous 3,600 image data set
- use two “master” files to map from this to a view of $2 \times 180^\circ$ sets — should be transparent to tools e.g. XDS

Multi-trigger / multi-sample

- Motivation: VMXi — in situ plate automated data collection
 - time / sample \sim 1-2 seconds
 - detector arming \sim 7 seconds
- Implement as: arm once, N triggers, each trigger for a 20° data set on separate volume
- each set logically distinct, though they share experiment metadata (wavelength, geometry, ...)



Multi-trigger / multi-sample

Collected data set: [0][1][2]...[N]

		^	^	^		^
master 1	-----+					
master 2	-----+					
master 3	-----+					
master N	-----+					

- Present as N master files, each mapping to a view of a 'distinct' data set
- can guarantee that this will confuse users sometime
e.g. 20 master files presented with only two data files?

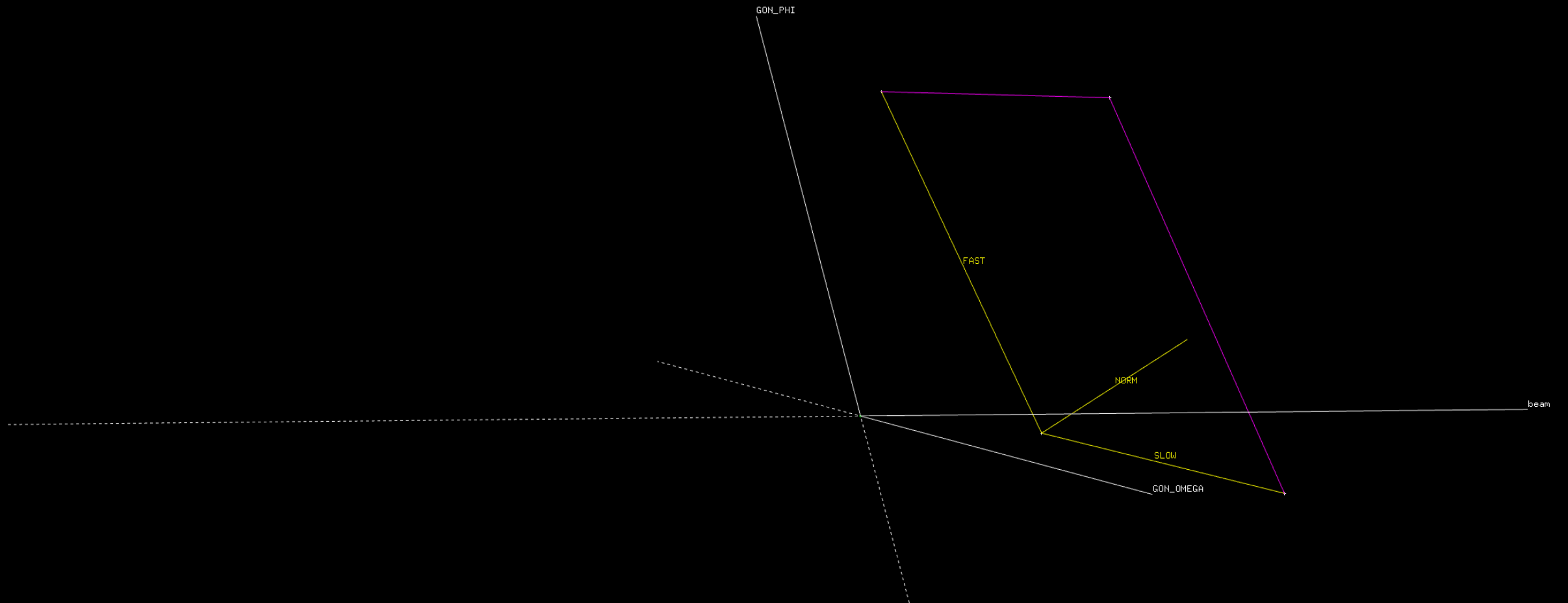
Consumer

NeXus is not a write-only file format

DIALS: geometry

- supporting file formats is expensive
- mix of proper geometry i.e. with depends_on attributes and beam centre / distance makes things fragile and cumbersome
- current support in DIALS limited to “standard” experimental geometry (it turns out)
- part of preparation for use of NXmx on chemical crystallography made example files, turns out support for e.g. 2θ axis broken

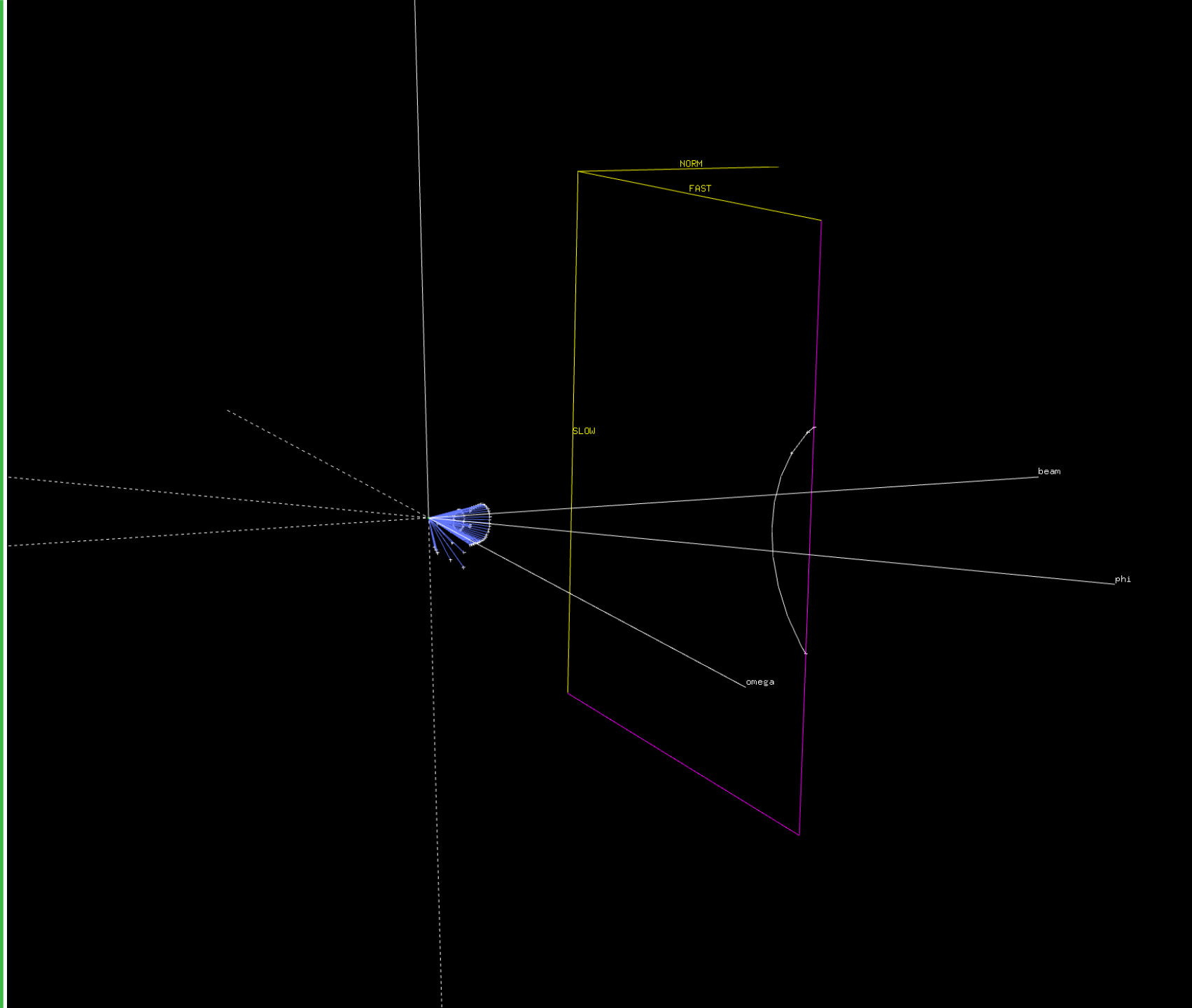
DIALS: geometry



DIALS: shadows

- computing of goniometer shadows done in processing from “prior knowledge” encoded in xia2 and DIALS (similar in autoPROC) — should this be the case?
- would be great to have shadow calculation done in DAQ software rather than every time data are processed

DIALS: shadow s



DIALS: NXmx

- would be great to have exactly one standard with no dialects, no variants — however unlikely to reach this point
- work in progress: we are building detector based on TIMEPIX which will use NXmx — we need to support non-Eiger data sources

Future

- NXmx is heading in a good direction
- gold standard is very helpful
- agreement on more features needed — we could be using GitHub more e.g.

<https://github.com/HDRMX/NXmx/issues/1> and

<https://github.com/HDRMX/NXmx/issues/2>

Request

- please can we have a place to store and critique example data sets to arrive on concrete conclusions of “these files are correct” or not — necessary to have different people produce and consume files for this — upload to zenodo, make issue in HDRMX / NXmx?

```
dials.import foo.nxs
```

```
dials.geometry_viewer imported.expt
```

```
dials.image_viewer imported.expt
```

- please try and if it fails or disagrees, complain! Software has bugs

Acknowledgements

- Controls team at DLS — Eiger integration with EPICS, ODIN, ...
- DAQ team — creating NeXus files, writing Durin
- Analysis crew inc. DIALS — supporting users at Diamond and elsewhere on working with the data
- EU, Wellcome trust, NIH, Diamond Light Source, CCP4 for support of DIALS

NXmx at DLS

Diamond unusual —

- Producer and consumer — GDA_o / xia2 & DIALS
- Biological and chemical crystallography
- Use NeXus extensively outside of MX and beyond Eiger detectors
- A central store of example data would be useful
- A forum for discussion of issues (GitHub) is very helpful —

we should use it!