Live Eiger Analysis with HDF5 & SWMR

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Acknowledgements

Controls: Emma Dixon, James O'Hea, Gary Yendell

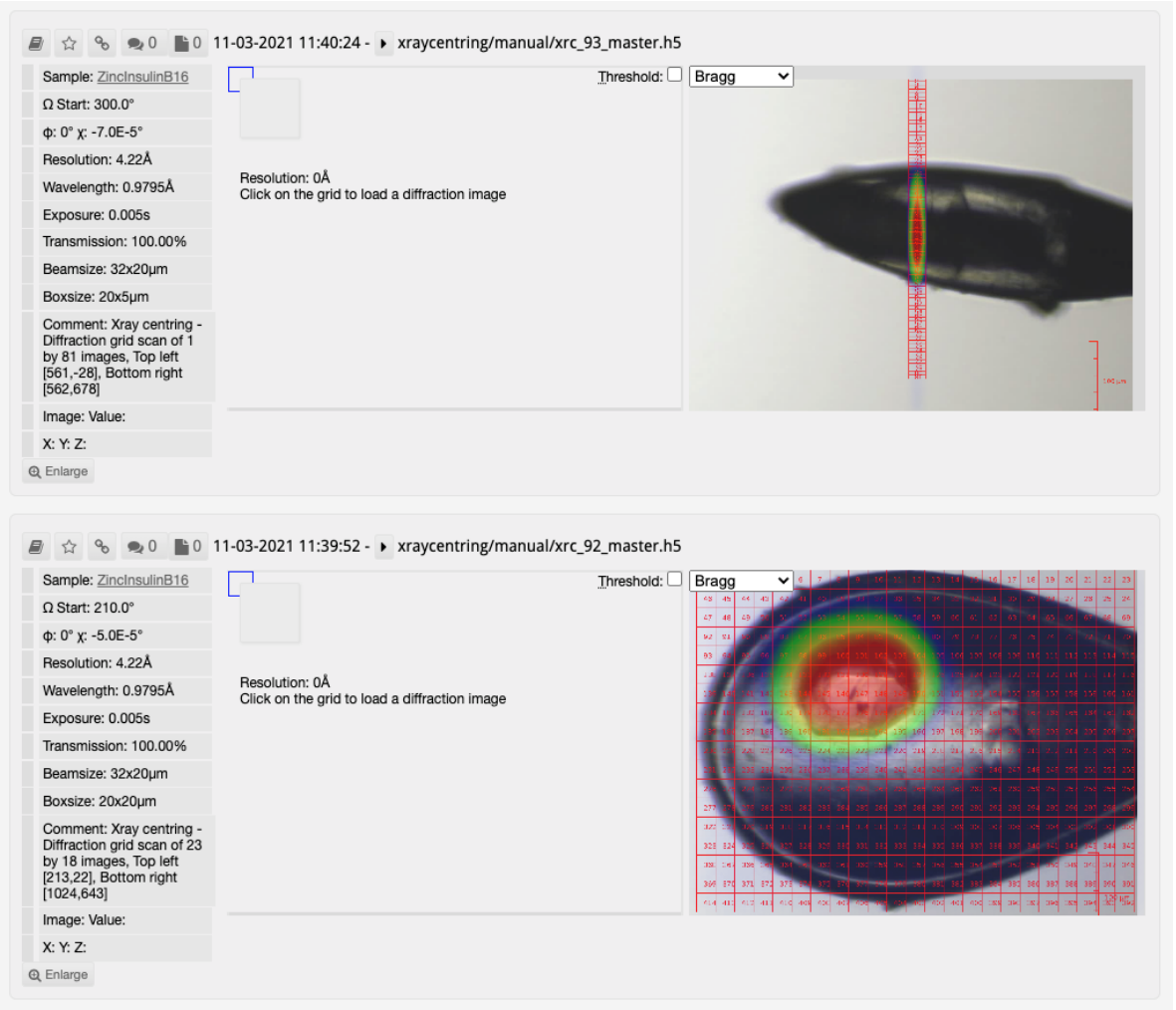
Data Acquisition: Chris Kelley, Paul Coe, Neil Smith

Data Analysis: Richard Gildea, Markus Gerstel

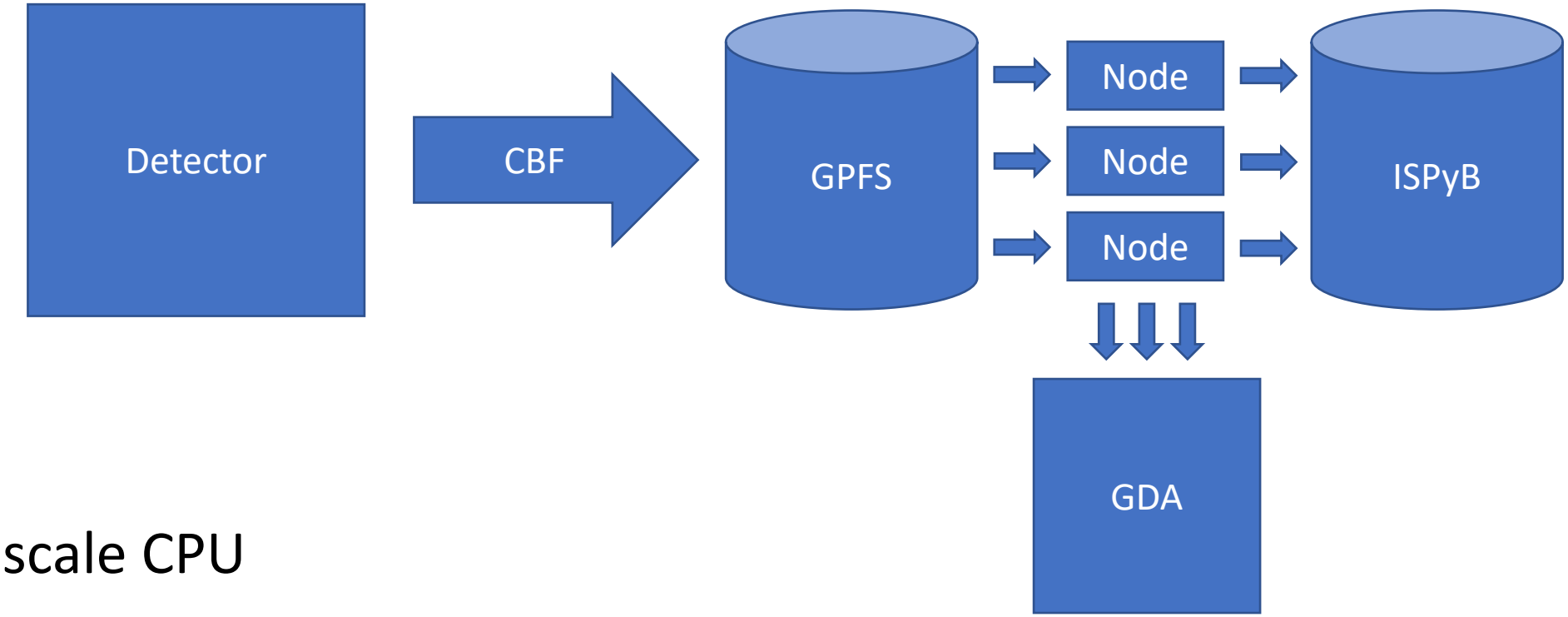
Infrastructure: Dave Bond, Rich Lear, Frederik Ferner

Beamlines: Ralf Flaig, David Aragao, Neil Paterson, Dave Hall, Danny Axford, Robin Owen

Only talking about grid scans!



Challenge : giving live feedback (Pilatus)



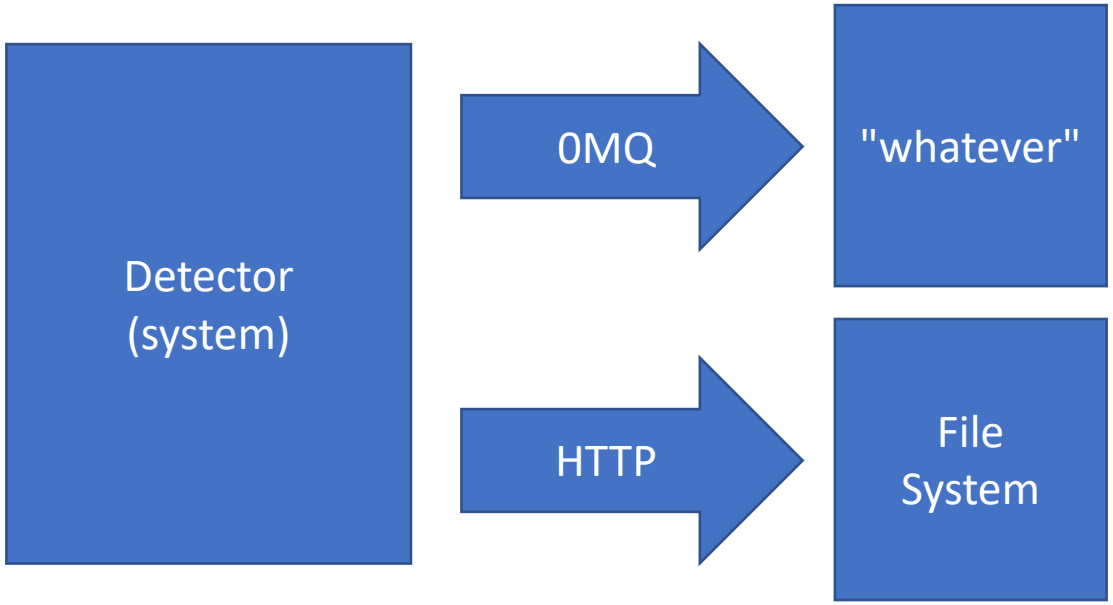
Nice:

- Can scale CPU
- Can analyze during acquisition

Nasty:

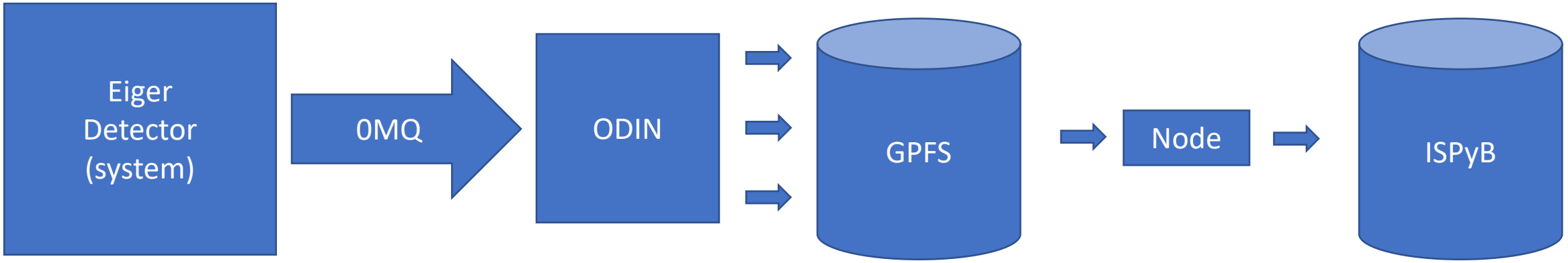
- GPFS dislikes 1000's of small files

Eiger: default configuration



- 0MQ allows you to do what you like
- File writer gives you finished data

Diamond configuration (late '18)



Nice:

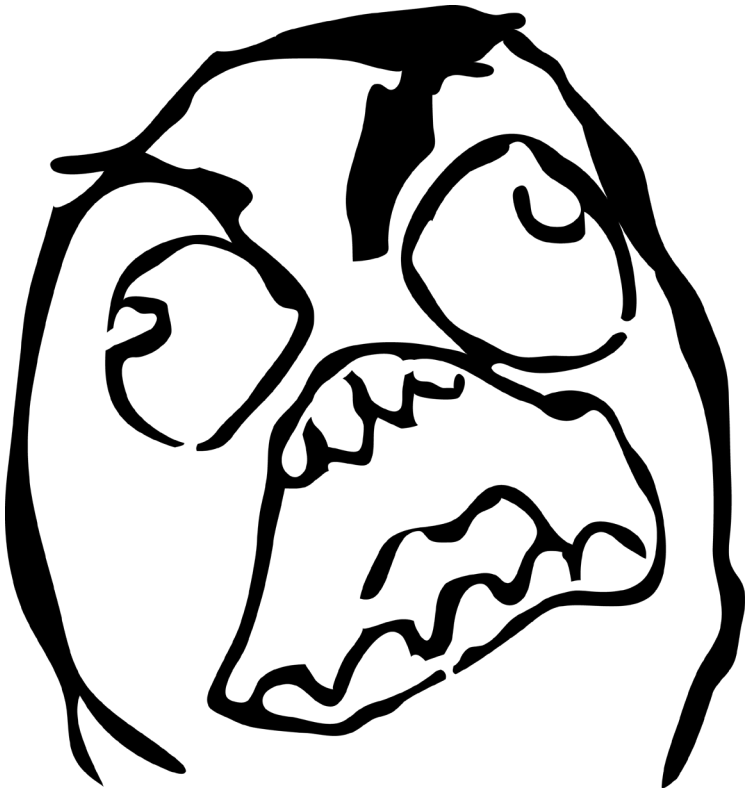
- Can acquire "flat out" for quite a long time – what we had on VMXi

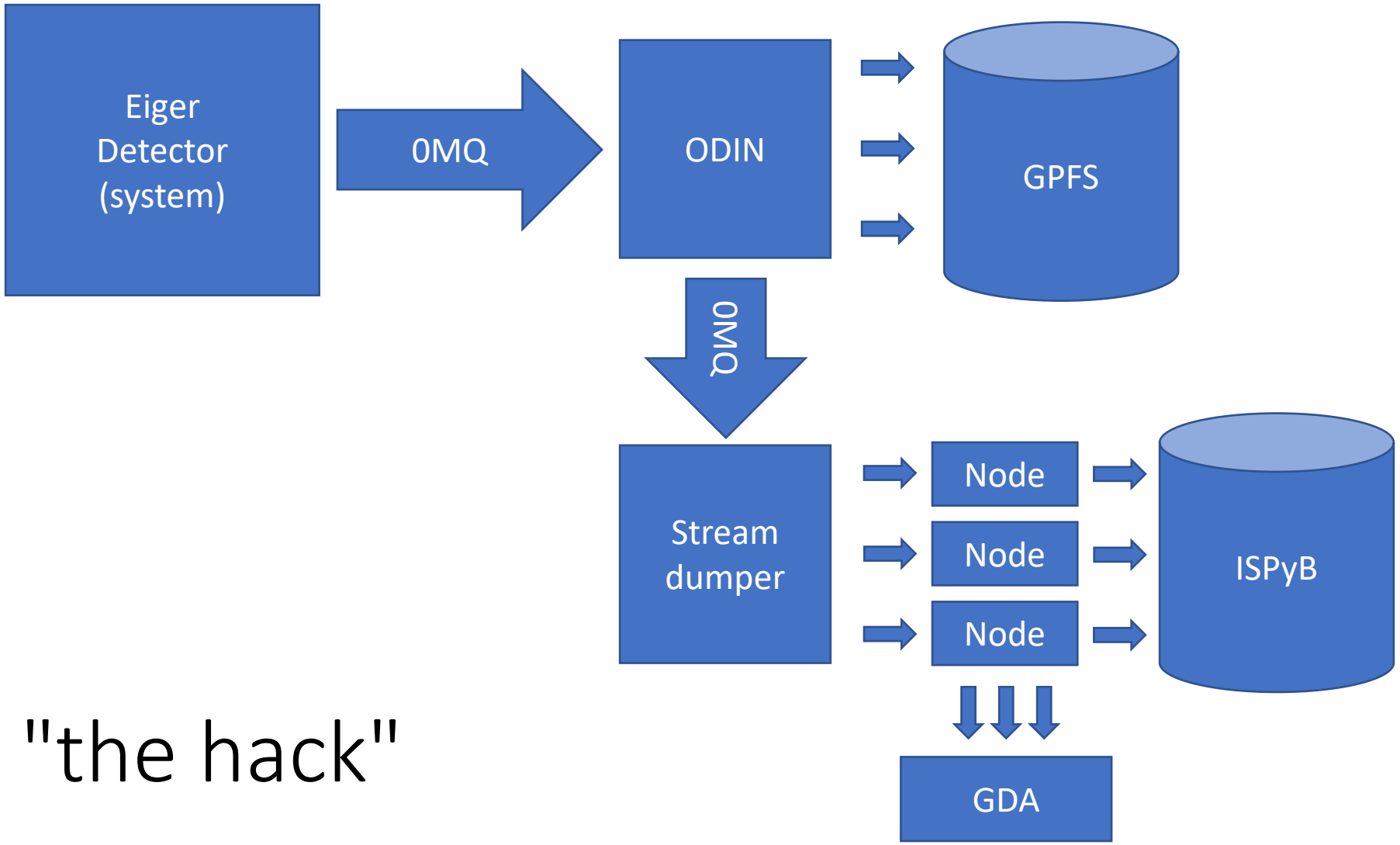
Nasty:

- Hard to analyze data during collection
- Data processing at end limited to one node (HDF5 1.8)

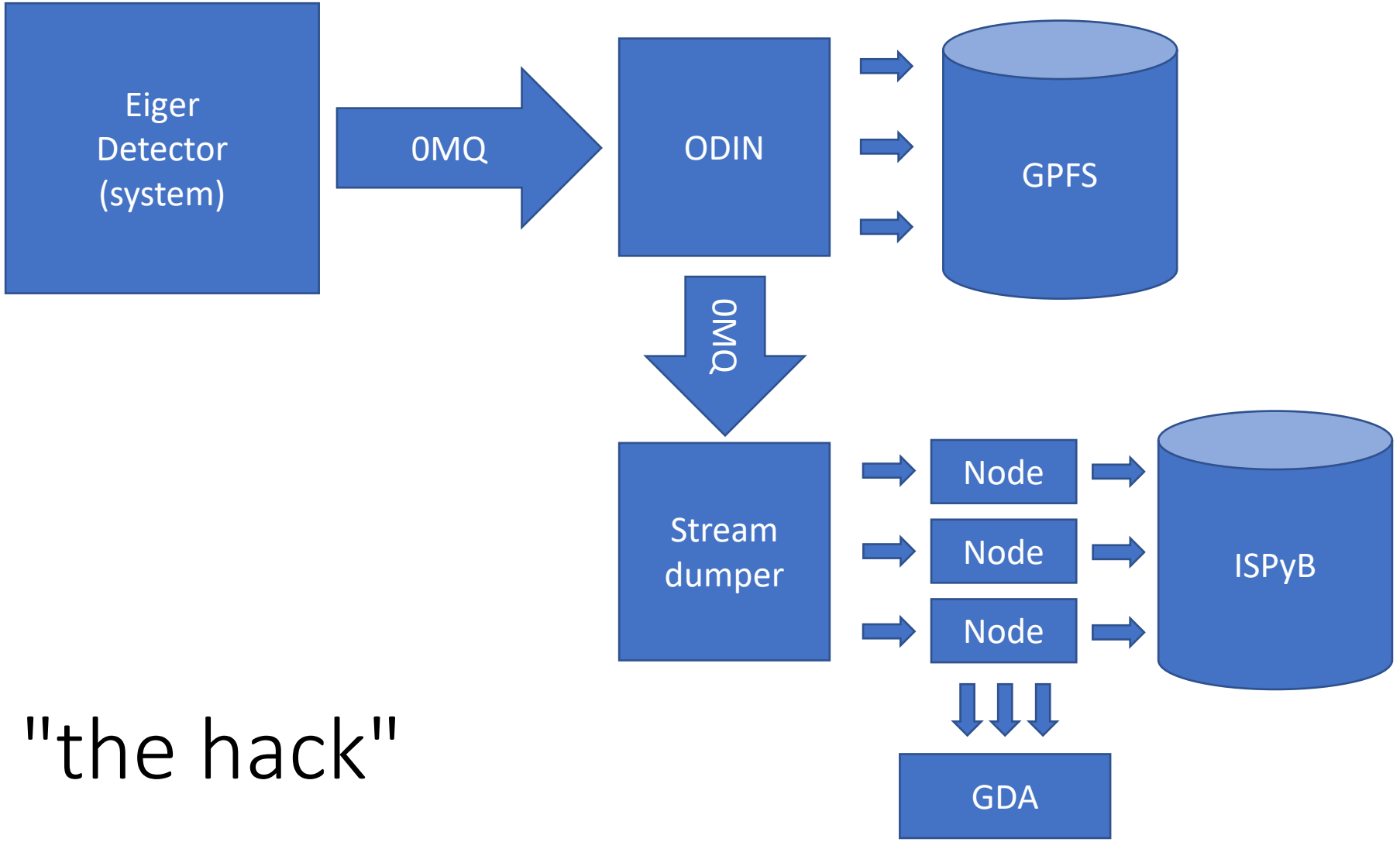
User feedback…

- Not favorable
- Per-image analysis for grid scans at end of collection big problem for big grid scans
- Retrograde step compared with previous detector systems
- "560 Hz Eiger 2XE slower than 100 Hz Pilatus"
- This feedback was *not wrong*




Eiger
Detector
(system)
0MQ
ODIN
GPFS
0MQ
Stream
dumper
Node
Node
Node
ISPyB
GDA

"the hack"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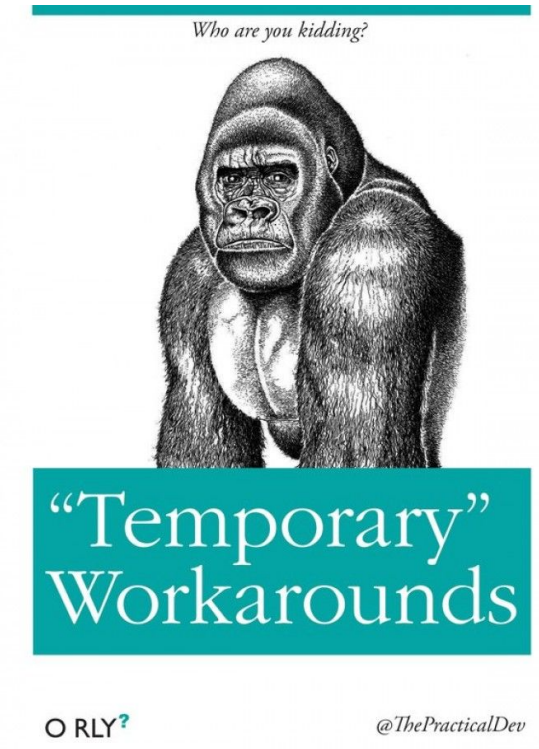

Who are you kidding?
"Temporary" Workarounds
O RLY?
@ThePracticalDev

"the hack" - qualities

Nice

- Can acquire data "flat out" but briefly e.g. 1,500 – 2,000 frames
- Can use CBF parallel infrastructure
- Can analyze during acquisition

Nasty

- Extra load (~ doubled) on file system
- Limited to 2,000 frames or so – no good for SFX

Key point: it *WORKED* and this hack was in production for 2 years

Meanwhile...

- HDF1.10 became commonplace in the wild
- Features added to HDF5 1.10.5 to check chunk size
- 1.10.5 features in h5py 3.0+ (rather recent)
- Push for SSX with Eiger

… time to revisit live analysis

SWMR, VDS, HDF5

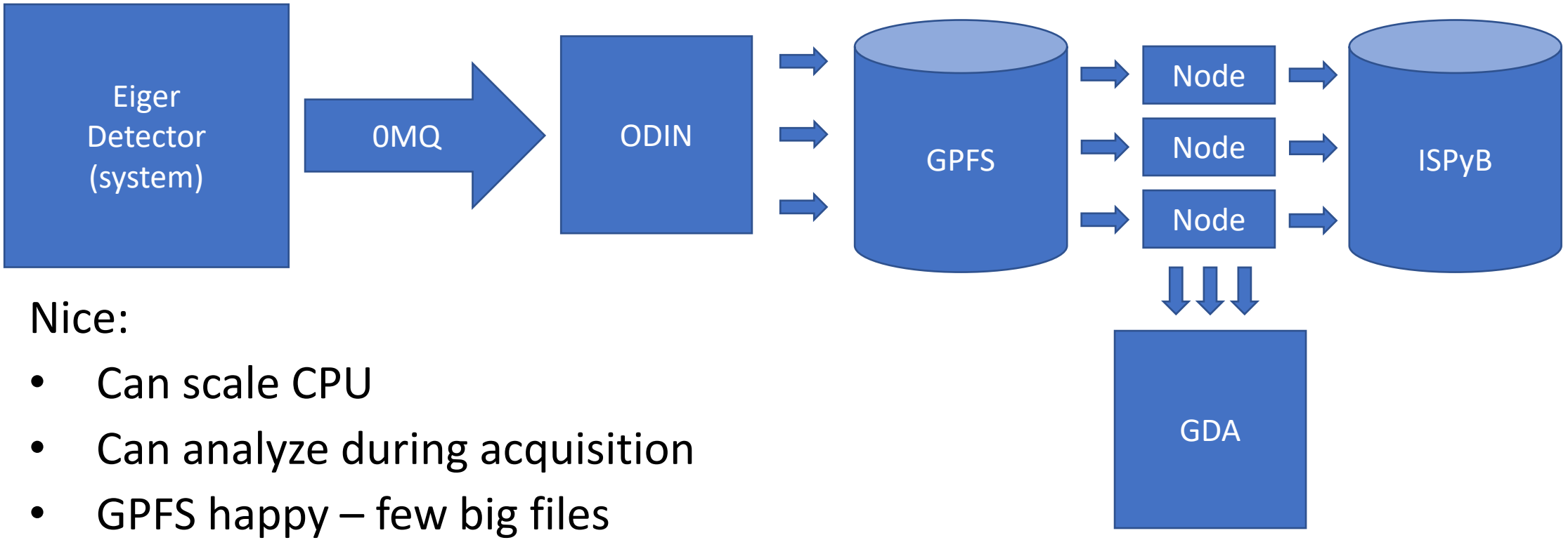
SWMR, VDS

- SWMR – single writer, multiple reader -> treat the HDF5 file as a directory, add "files" to it (i.e. add chunks to a dataset)
- VDS – virtual data set – define /entry/data/data to *look* like a real data set but it points into data_000001.h5 etc.

Using SWMR and VDS

- Master file defines VDS -> we know what images will appear
- Data files written as SWMR from ODIN
- Extension to "file watcher" to
  - Watch for appearance of data_00000N.h5
  - Watch data_00000N.h5 for appearance of frames (i.e. size > 0)
  - Trigger analysis on logical frame (i.e. map from real chunk ID in data_00000N.h5 to N00j)

Diamond configuration



Nice:

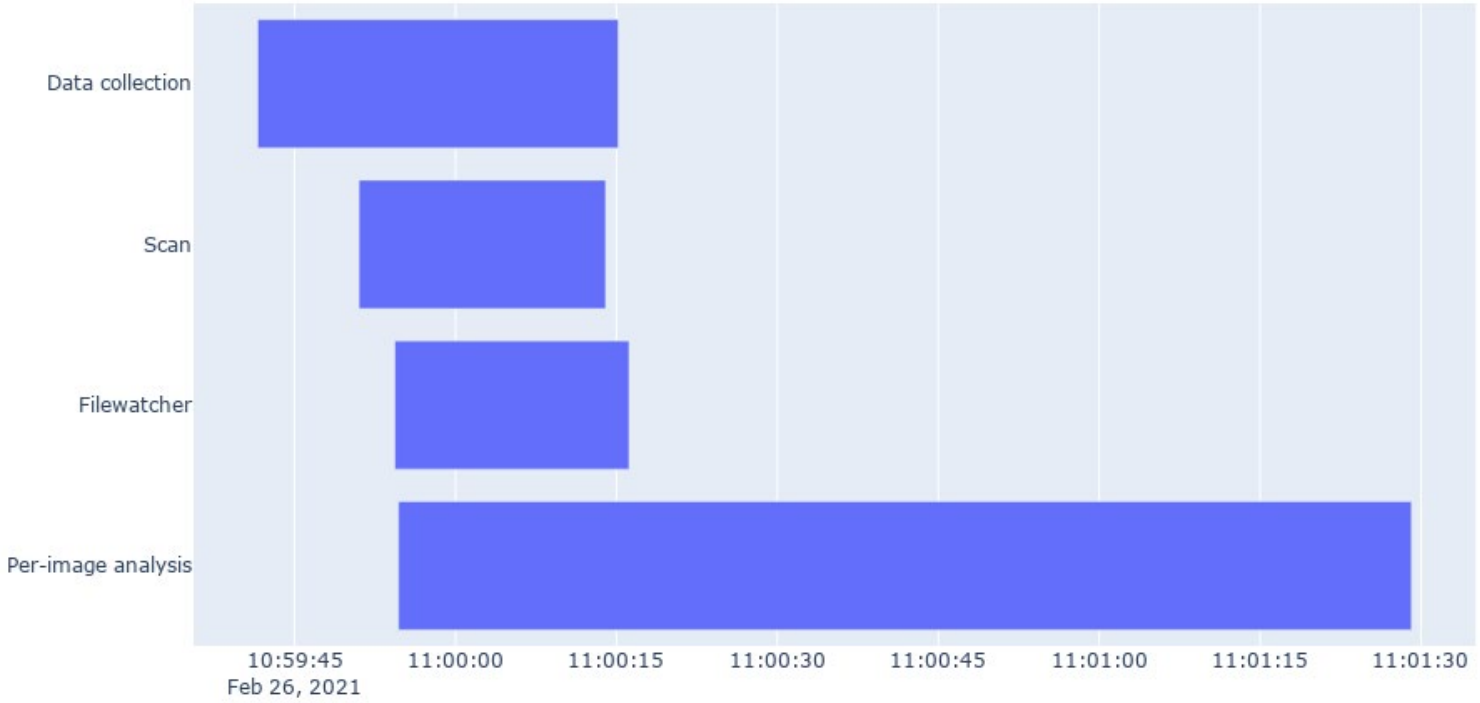
- Can scale CPU
- Can analyze during acquisition
- GPFS happy – few big files
- No real limits

Nasty

- No real limits

Example case i04 Eiger 2XE 16M

- 86x73 grid scan – 6,278 x full 16M frames @ 1.99ms exposure
- 1 image per trigger on position readback



Scan took 22.3s

Real-world ~280 Hz

File watching latency ~ 3s


YOU'RE GOING TO NEED
A BIGGER ~~BOAT~~ CLUSTER

800 cores... not a whole cluster but...

Processing 6,278 images < 22s -> can keep up in real-time

09:54:21.715 - filewatcher started watching

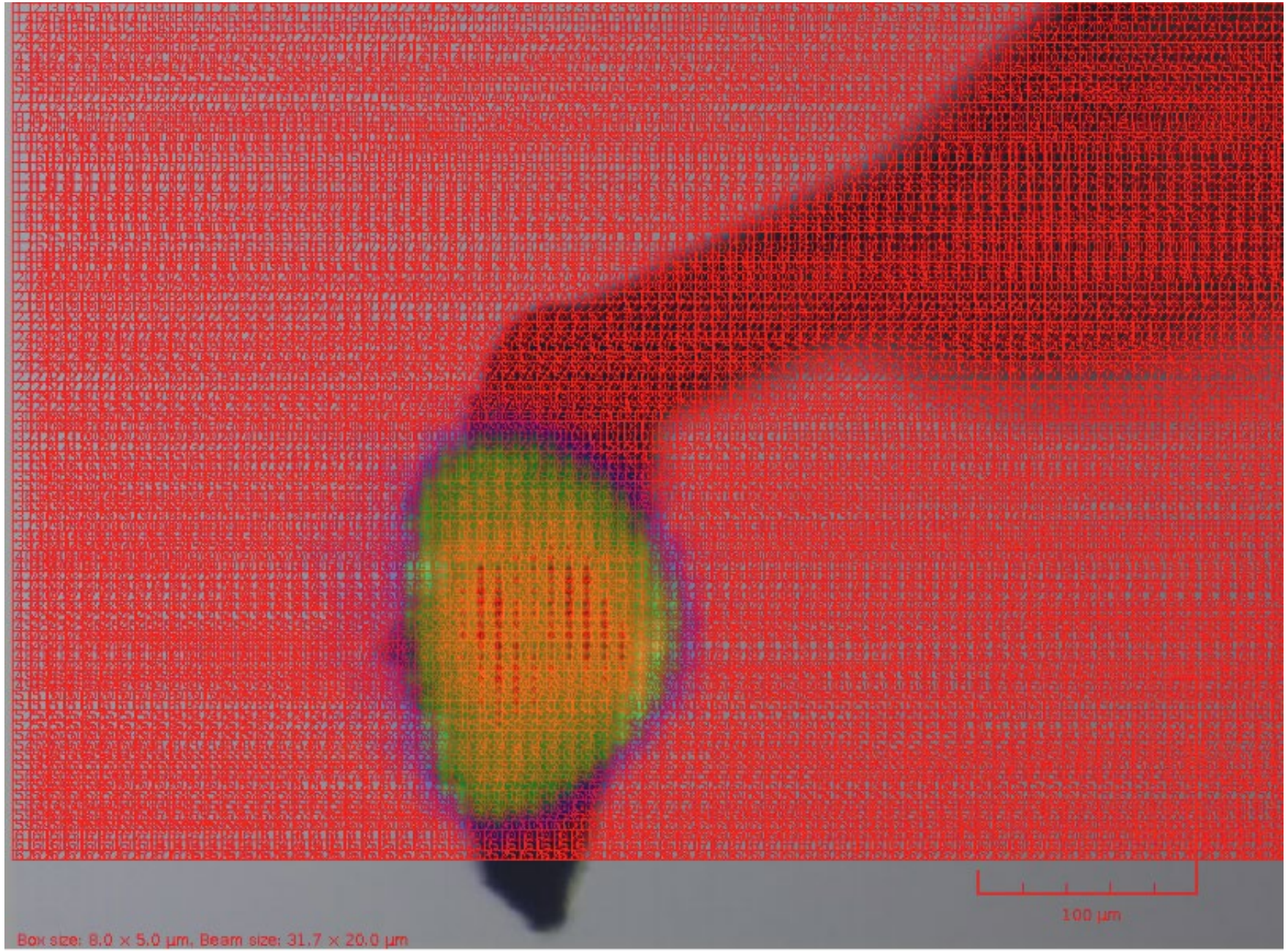
09:54:31.657 - filewatcher found all images

09:54:21.811 - PIA started on first image

09:54:43.685 - PIA on last image

However…

SWMR does not fix everything



Discussion

- HDF5 better solution in long term than e.g. dumping CBF files – for i04 example 6,278 frames were 108GB in CBF format, 10GB in HDF5
- Far fewer files (~3 orders of magnitude) - happy GPFS
- Can easily keep up acquisition as fast as detectors can do
- Removed limiting factors on grid scan size -> need to provision more analysis resources
- All of the software (ODIN, dials etc.) open source so this should all be available
- Making the spot finding more compute efficient on our to-to list

Comments

- Removing limitations on what we can do with the detector highlights other issues e.g. processing resources etc.
- Displaying analysis for O(10k) and greater grid scans will require thought
- SWMR, VDS and HDF5 *appear* to be stable in production on MX beamlines at Diamond
- We can only do this because we have Eiger 2 XE, ODIN, 40 Gb network, GPFS, infiniband in cluster, … the software is only part of the solution
- Given the compute resources no obvious blocker for ~ real time analysis