ISPyB
at Diamond

Neil A Smith

ISPyB Meeting 31st January 2018

- Beamlines

- Status

- Future plans

ISPyB Updates: Support to Beamlines

Cryo-EM
Data collections recorded in ISPyB
Collaboration with ESRF on Scipion
based workflow

MX
DHL automated shipping integration
More statistics and reporting
Integrated zocalo processing
architecture – **Graeme's talk**

XPDF
Mapping workflow and concepts
against existing database tables
Tim's talk

VMXi
UI improvements for crystal selection
More meta data in ISPyB e.g.
crystallisation screens
Juan's talk

Xchem
Recent requirement
Increasing experiment throughput by
use of multi-pin sample holders
Alice's talk

Lots of incremental improvements…
Lots of requirements too…

diamond

ISPyB at Diamond: System architecture

ISPyB database – clustered solution

Maria DB solution with Maxscale proxy

Main web application and services
provided by SynchWeb

Mobile app developed and supported by
bespoke web services (SynchLink WS)

Stats:
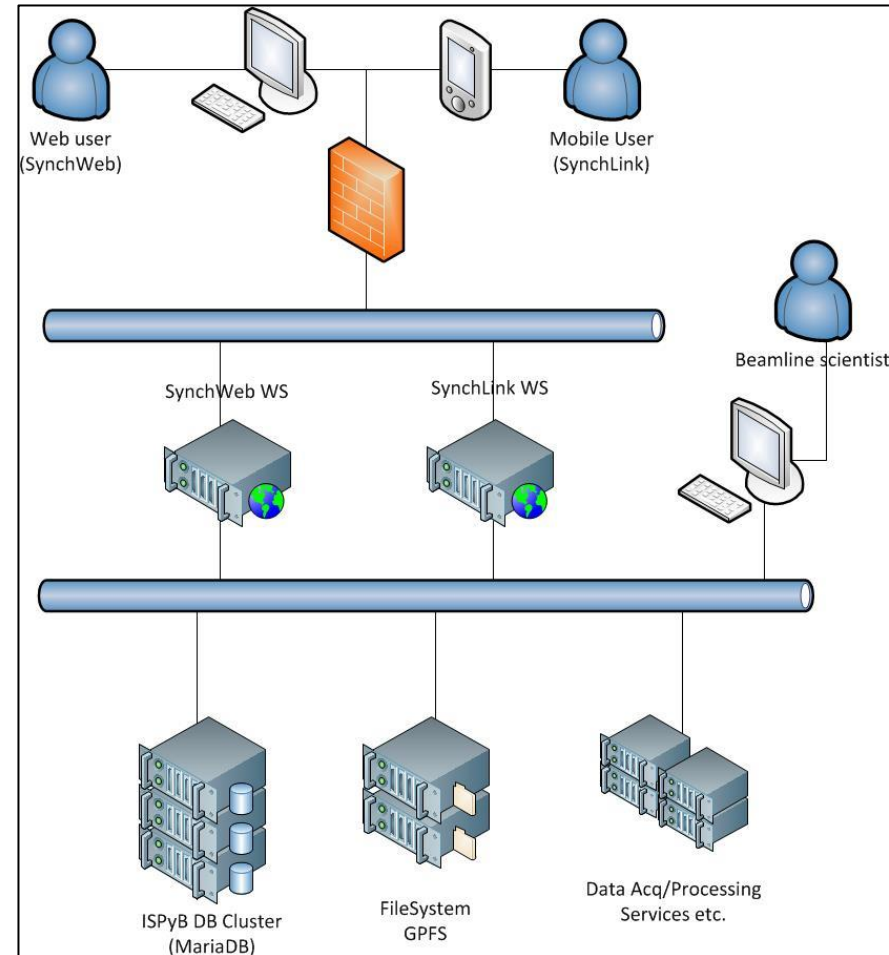 1,000-1300 unique users / month
  8,000 – 10,000 page views
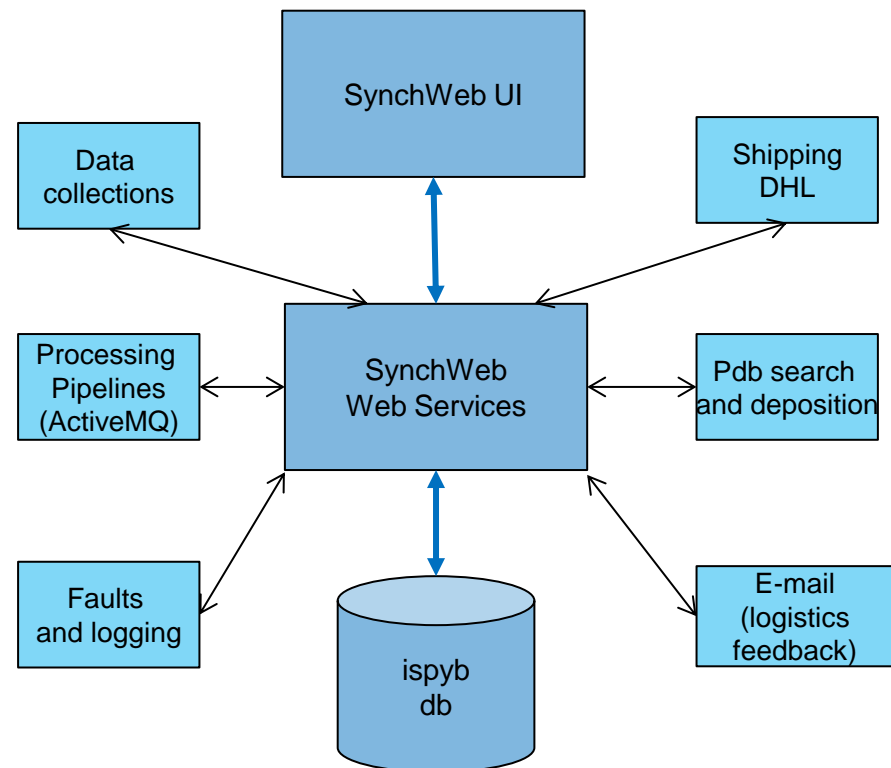 50% of users remote
  20,000 sessions
 7,000 proposals
  >1.3M data collections

ISPyB at Diamond: SynchWeb

- SynchWeb provides software stack to handle shipping, data collections etc.

- Integrates with Diamond processing pipelines and third party systems

- ~70k Javascript SLOC

- ~20k PHP SLOC

- All meta data stored in ISPyB database

ISPyB at Diamond: future plans for software
Migrate bespoke mobile services to ISPyB
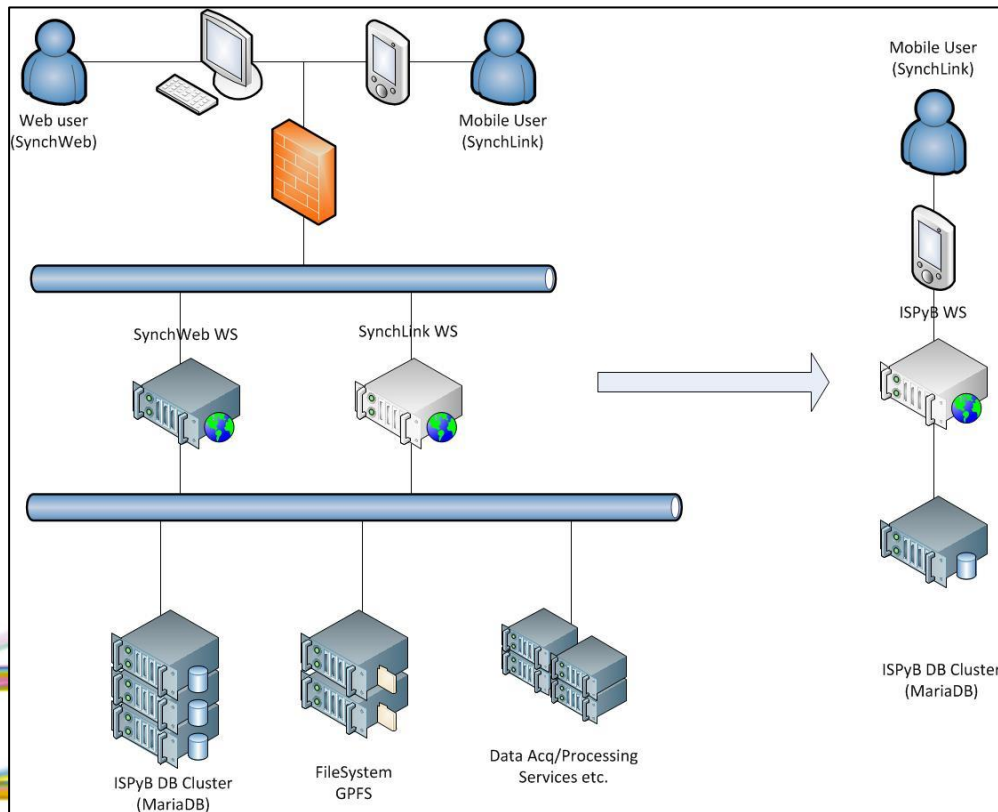
Replace bespoke web services with ISPyB WS

Investigated deploying as Wildfly SWARM application
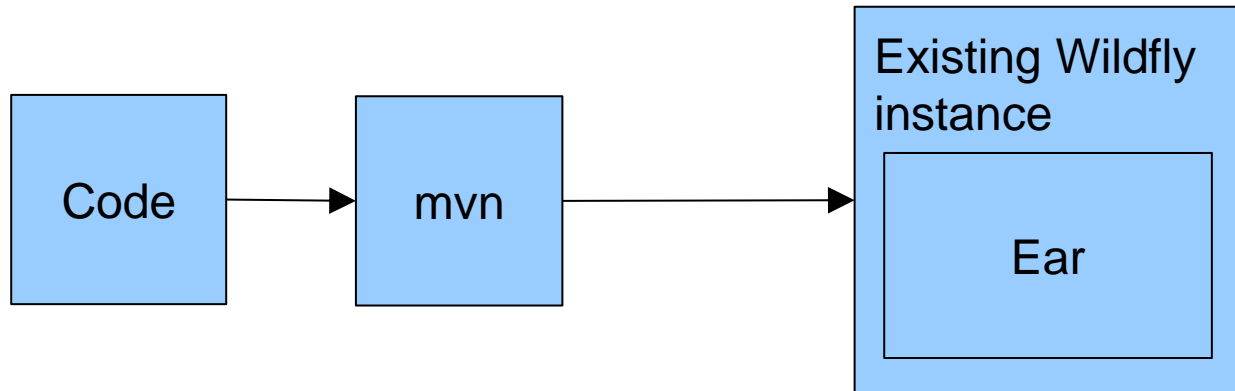
Simplifies deployment (single jar)

Can support scalability using ngnix proxy

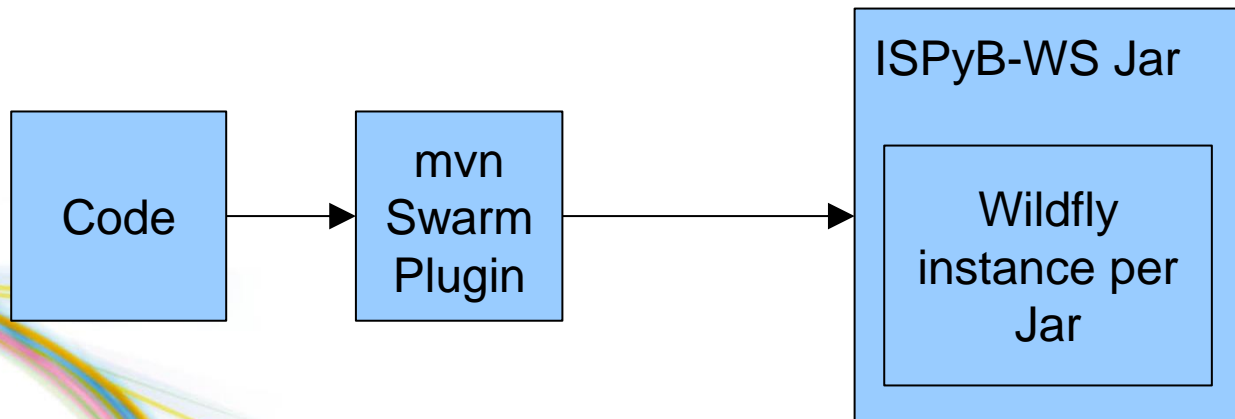Additional contractor brought in to develop ISPyB web services

ISPyB at Diamond: future plans for software
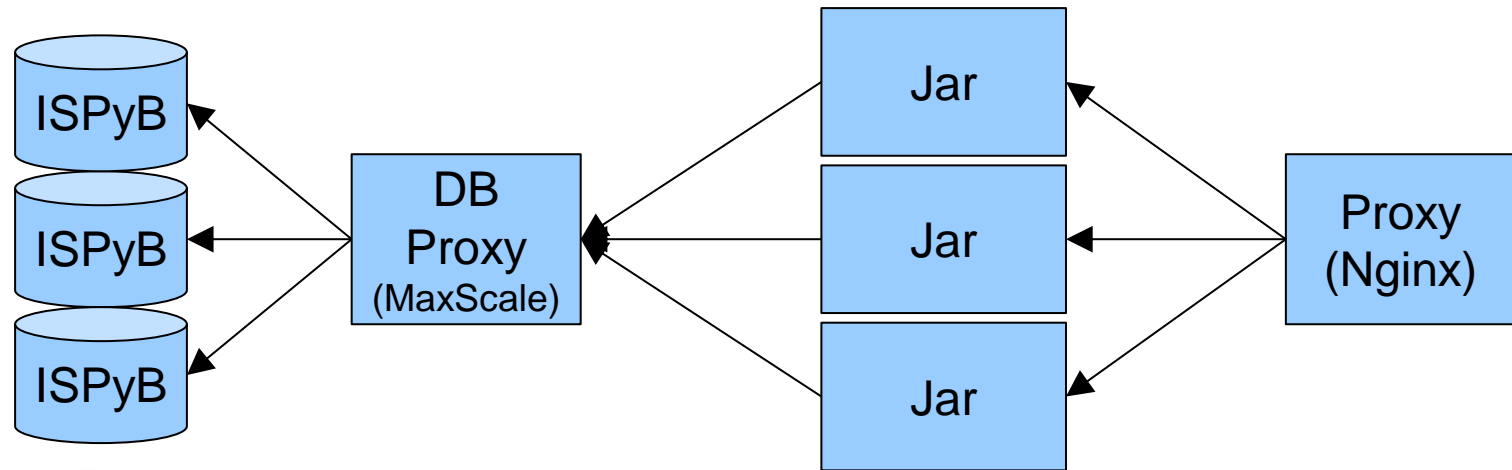Migrate bespoke mobile services to ISPyB

Wildfly 8

| Code | → | mvn | → | **Existing Wildfly instance** |
| | | | | Ear |

Wildfly 10

| Code | → | mvn Swarm Plugin | → | **ISPyB-WS Jar** |
| | | | | Wildfly instance per Jar |

https://github.com/belkassaby/ISPyB/tree/wildfly-swarm

diamond

# ISPyB at Diamond: future plans for software
Migrate bespoke mobile services to ISPyB

ISPyB at Diamond: Summary

- ISPyB is the core of our LIMS and used heavily

- Looking to reduce number of bespoke software solutions supported

- Need to move fast but not diverge

- Large number of database modelling issues (Karl will brief later)

- Recommend holding monthly webex meetings to move discussions forward in developer community

- Need to clarify approval process

- Do database changes need ratification from steering or science committee?
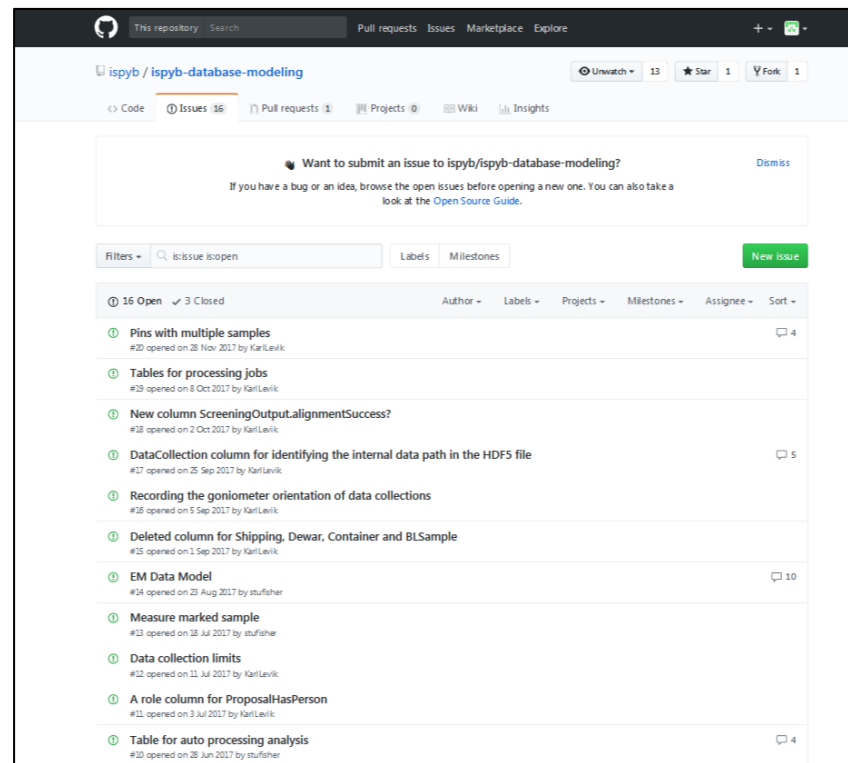
ADDITIONAL SLIDES

SynchWeb Updates

Stu Fisher
DLS Contractor
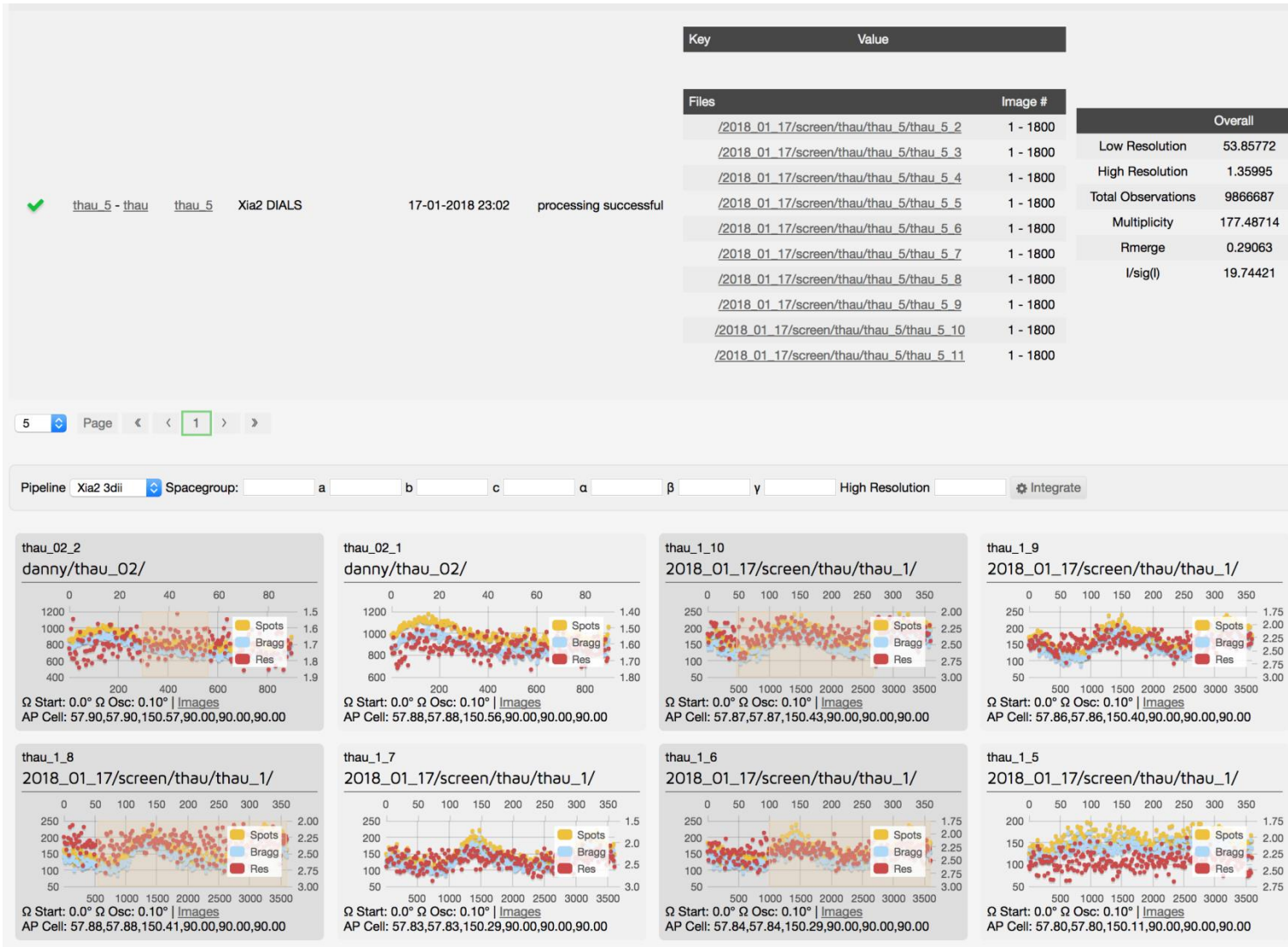Quantum Detectors

ISPyB Meeting DLS
January 2018

Zocolo Reprocessing Architecture

- Allows job monitoring from DB
- Simplified interface for re-integrating data sets

Zocolo Reprocessing Architecture

- Reworked multi crystal integrator
- Showing input parameters, status, and merging statistics
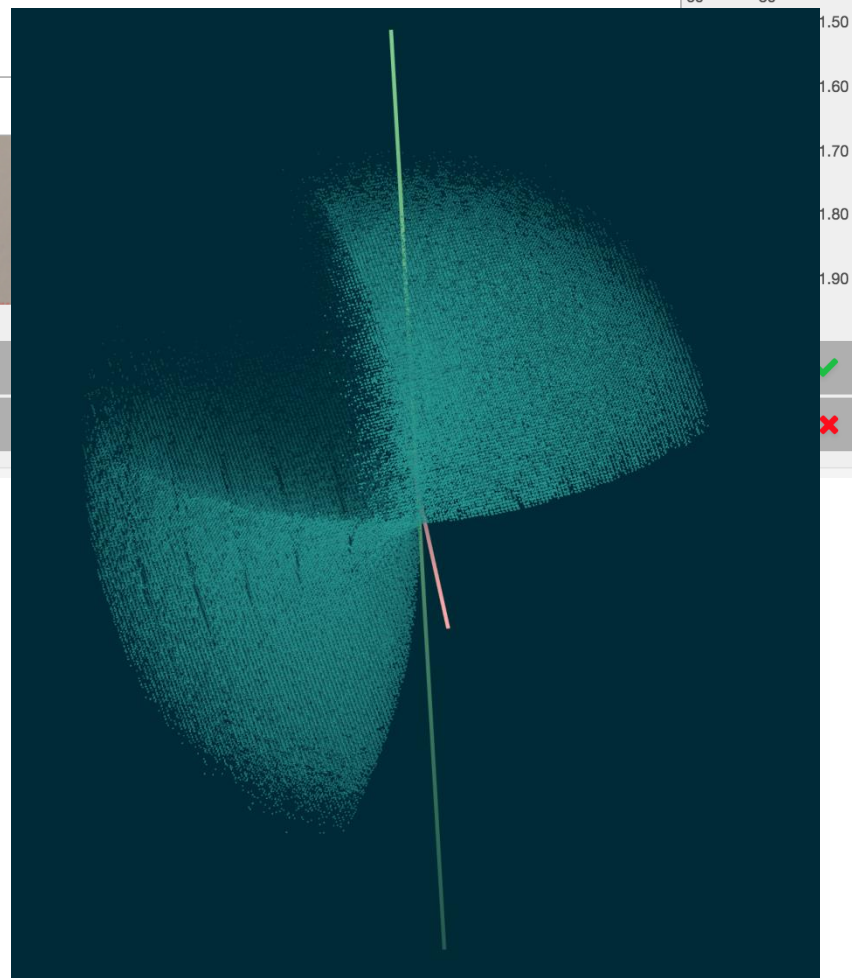
DataCollection Attachments

- Now adding reciprocal space output to each data collection
- Integrated reciprocal space viewer (uglymol)
- Could easily be extended to store other data collection specific attachments (not processing)

DHL Integration

- International and domestic users can automatically create airway bills and book pickup
- International users get quoting system

- Print pdf airway bill from SynchWeb

- Automatically fills in tracking numbers so staff / users can track where dewars are

- In use at DLS for around 6 months.

Create Airway Bill: To Facility

Shipment Details

Shipment	test
Dewars	☑ Dewar1
Weight	18 Kg
DHL Account Number	Click to edit
Declared Value	100 GBP
Package Description	Dry shipper - not restricted as per IATA special provision A152

Contact Details

Contact	Spring 8
Contact Phone Number	1234567890
Contact Email	test@spring8.co.jp

Laboratory Details

Laboratory Name	Spring8
Laboratory Address (excluding post code)	1-1-1, Kouto, Sayo-cho, Sayo-gun
Laboratory City	Hyogo
Laboratory Postcode	679-5148
Laboratory Country	Japan [Free For: United Kingdom]

Pickup Details

Package Location Location where shipment can be picked up from	stores
Shipping Date	31-01-2018
Ready By Time shipment will be ready for pickup	15:51
Close Time Time after which shipment cannot be picked up	20:51

Quotes

	Product	Delivery	By	Cut Off Time	Booking Time	Price
●	EXPRESS 12:00	05-02-2018	12H	18H	17H30M	303.46
○	EXPRESS WORLDWIDE	05-02-2018	23H59M	18H	17H30M	317.8

EXPRESS WORLDWIDE ECX DHL
2017-07-21 XMLPI 6.0 / *90-1604*
From : University College Dublin
last name
Belfield
4 Dublin
Ireland, Republic Of   Origin: DUB   Contact: 12345
To : Diamond Light Source
John Peychers
Fermi Avenue
OX11 0DE Didcot
United Kingdom   Contact: +44 (0)1235 778787
EMGW **GB-OXF-OXF**
Day   Time
Ref :   Pce/Shpt Weight   Piece   **18.0 kg 1/1**
Contents: Dry shipper - n ot restricted a s per IATA spec ial provision A 152
WAYBILL 92 4210 4443
(2L)GBOX110DE+51000000
(J) JD01 4600 0036 4893 5902

Dewar Overview and Tracking

Dewar Overview

This page shows all dewars for all current visits

i02   i02-2   i03   i04   i04-1   i23   i24

Imager Requested

First Experiment: 13-01-2018

Search

Start Date	Visit	Beamline	Local Contact	Shipment	Dewar Name	Dewar Code	Containers	Courier	Track # to	Status	Location	Tracking
19:00 13-01-2018	mx13467-53	i03	Mr Mark Williams	JIC_130118_I03	DLS-MX-0671	DLS-MX-0671	DLS-442, DLS-443	DHL	4407975401	at facility	stores-out	Delivery: OXFORD-GBR
19:00 13-01-2018	mx13467-53	i03	Mr Mark Williams	MX13467-53-i03-130118-UEA-AMH	DLS-MX-0012	DLS-MX-0012	DLS-201, CPS-3568, CPS-3569, CPS-3572, DLS-203	DHL	7542101350	at facility	stores-out	Delivery: OXFORD-GBR
12:00 13-01-2018	mx13587-59	i03	Mr Mark Williams	Durham mx13587-59	DLS-MX-0521	DLS-MX-0366	DLS-470, DLS-277, DLS-278, DLS-279, DLS-471	DHL	2255238845	at facility	stores-out	Delivery: OXFORD-GBR
10:00 13-01-2018	mx15916-36	i24	Dr Danny Axford	mx15916-36_Shipment1	mx15916-36_Dewar1		CPS-2318, CPS-2319, CPS-2317, CPS-2321, CPS-2309	Cambridge Courier		at facility	stores-out	
10:00 13-01-2018	mx15916-36	i24	Dr Danny Axford	DKforI24	DLS-MX-0614	DLS-MX-0614	DLS092, DLS093, DLS094, DLS095	DHL	1399419604	at facility	stores-out	Delivery: OXFORD-GBR
10:00 13-01-2018	mx15916-36	i24	Dr Danny Axford	Daniil Prigozhin	DLS-MX-0602	DLS-MX-0602	MRC-LMB-2, MRC-LMB-3, MRC-LMB-6	DHL	2419354184	at facility	stores-out	Delivery: OXFORD-GBR
10:00 13-01-2018	mx17221-11	i04-1	Mr Jose Brandao-Neto	mx17221-11Shipment1	DLS-MX-0217	DLS-MX-0217	CSB2-4, CSB2-5	DHL	3390118771	processing	stores-in	Delivery: OXFORD-GBR
10:00 13-01-2018	mx17221-11	i04-1	Mr Jose Brandao-Neto	mx17221-11_Shipment1	mx17221-11_Dewar1		DLS-672, DLS-0041, CSB1-4			at DLS		
10:00 13-01-2018	mx17221-11	i04-1	Mr Jose Brandao-Neto	mx17221-11Shipment1	DLS-MX-0578	DLS-MX-0578	CSB1-2, CSB1-3	DHL	3390118771	at facility	stores-out	Delivery: OXFORD-GBR

- Find out where dewars are for experiments on your beamline at a particular time
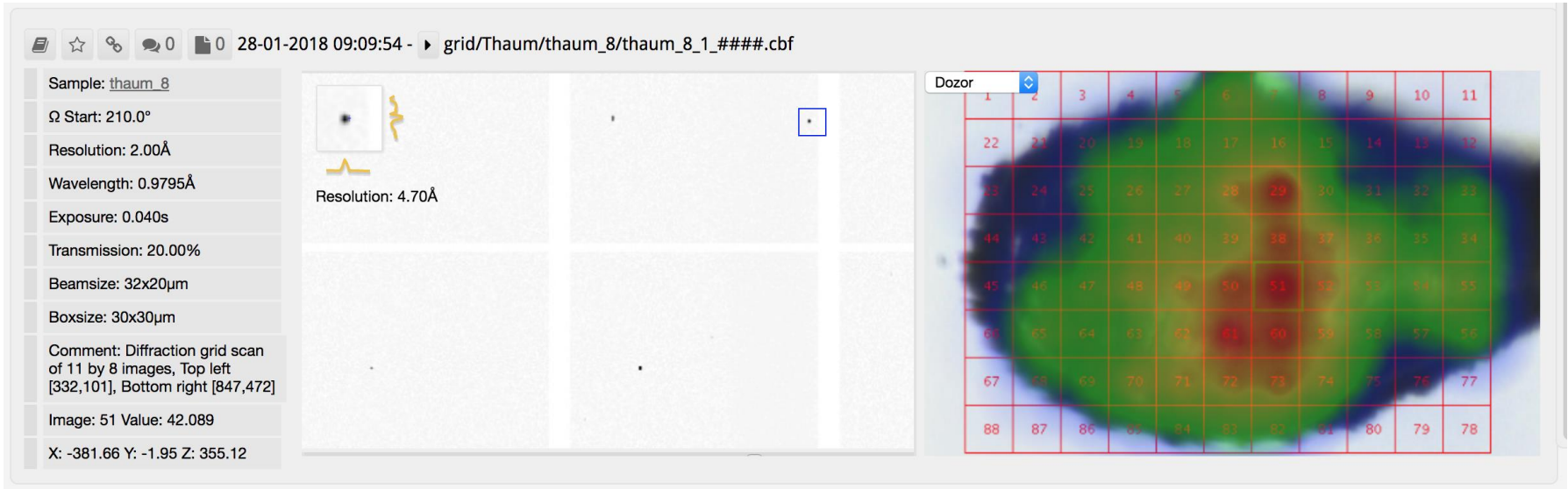- Because DHL api populates tracking details we have built in DHL tracking

Processing Graphs

- Finally have json for processing results from xia2, dials, autoproc

- Friendly interface where multiple processes can be plotted against each other and against multiple parameters
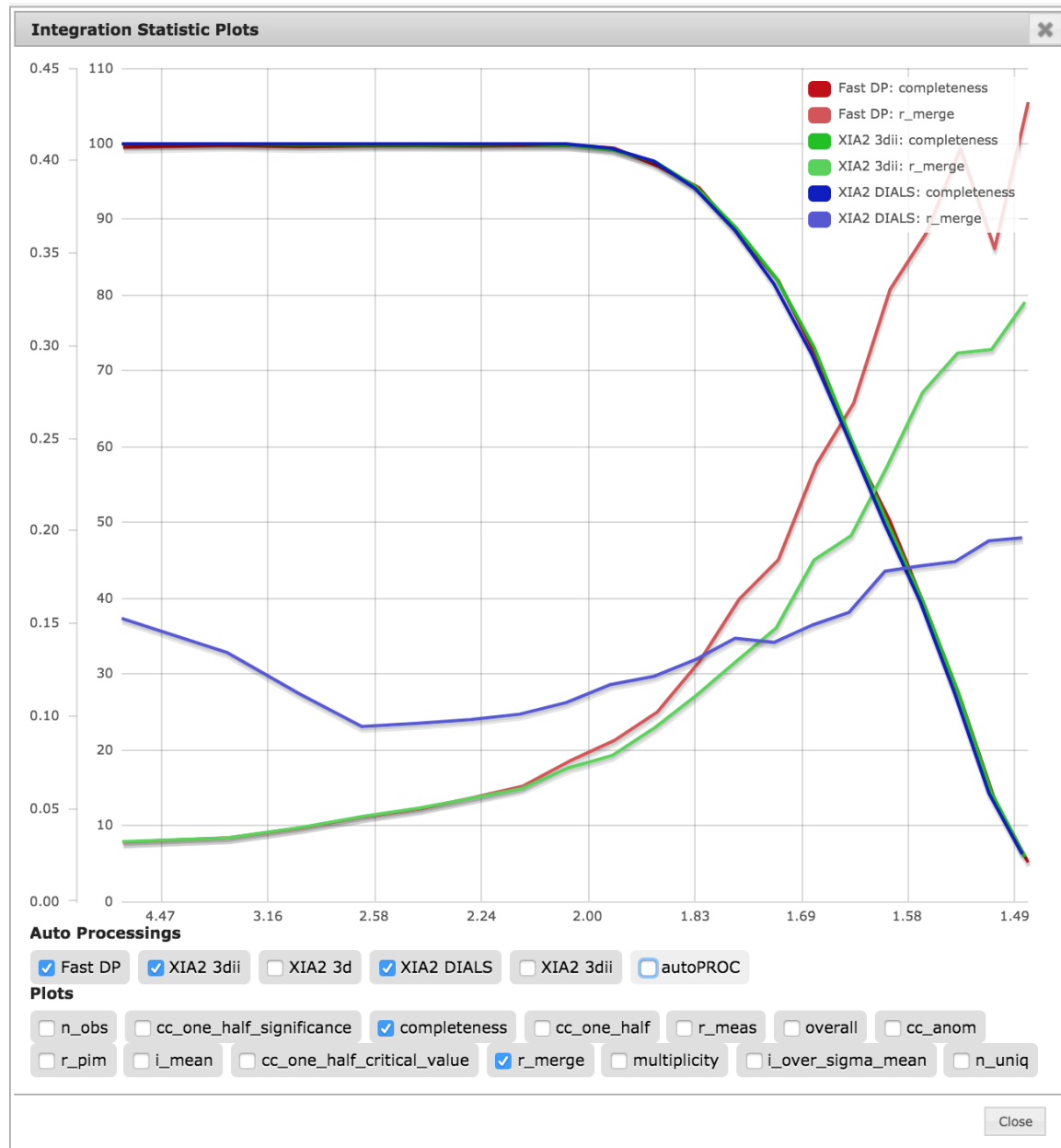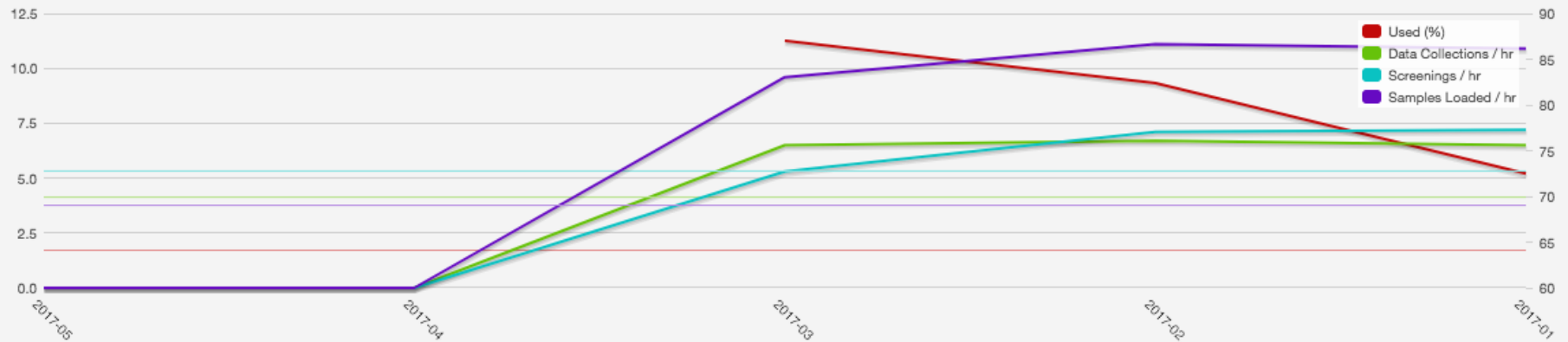
Grid Scan View

- Now have dozor image quality indicators results with grid scan view

Extensive Reporting Statistics

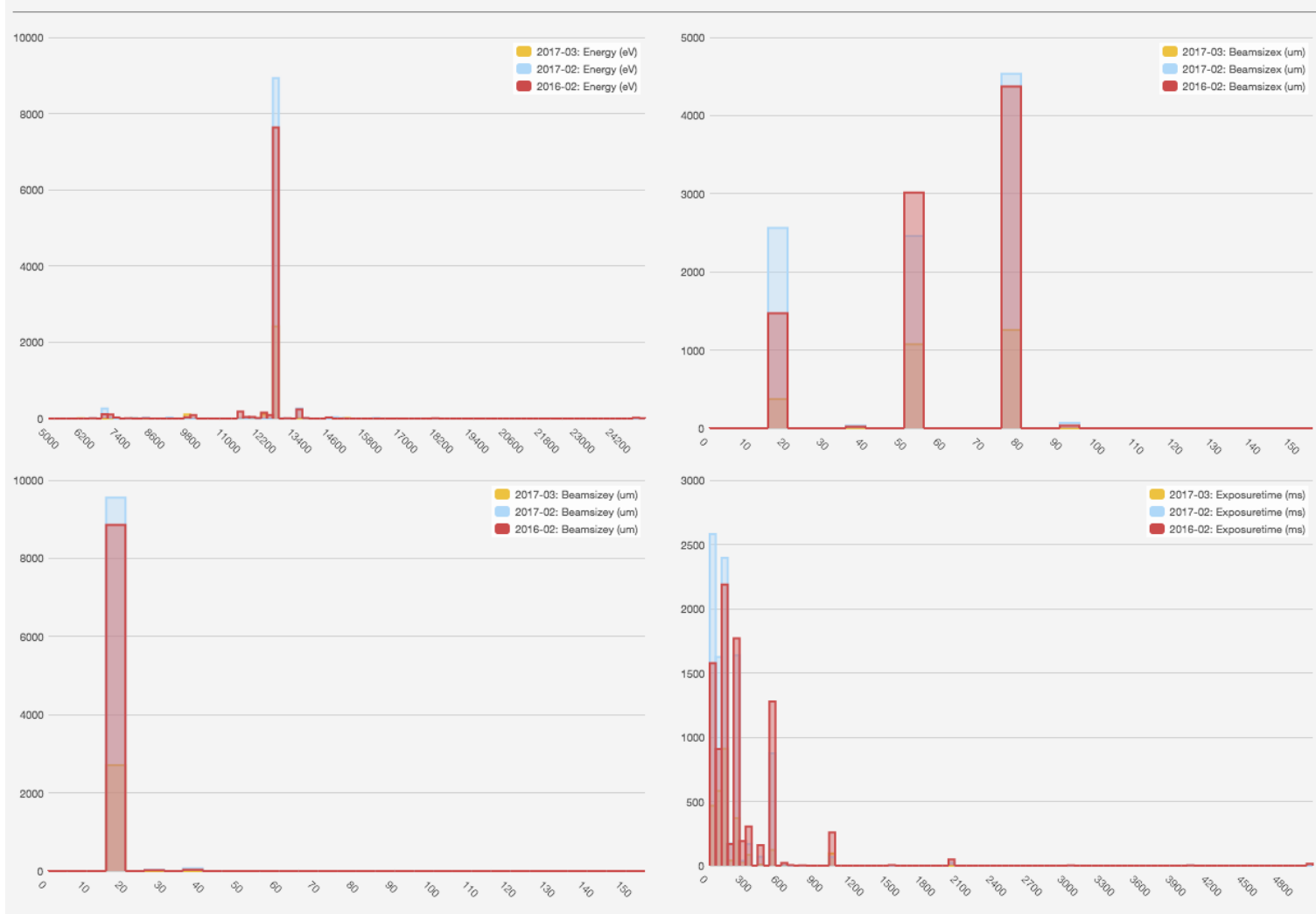|	Run	No. Visits	Allocated (hr)	Remaining (hr)	Used (%)	Data Collections / hr	Max / hr	Total	Screenings / hr	Max / hr	Total	Samples Loaded / hr	Max / hr	Total
☐	2017-05	1	8			0	0	0	0	0	0	0	0	0
☐	2017-04	28	359			0	0	0	0	0	0	0	0	0
☐	2017-03	59	705	92	87	6.5	33	1731	5.3	25	1415	9.6	25	2333
☐	2017-02	58	655	115.4	82.4	6.7	54	3659	7.1	40	3890	11.1	40	5828
☐	2017-01	72	2546	701.1	72.5	6.5	54	4538	7.2	32	5062	10.9	34	7473

- How has beamtime been allocated vs used over this run and the proceeding ones
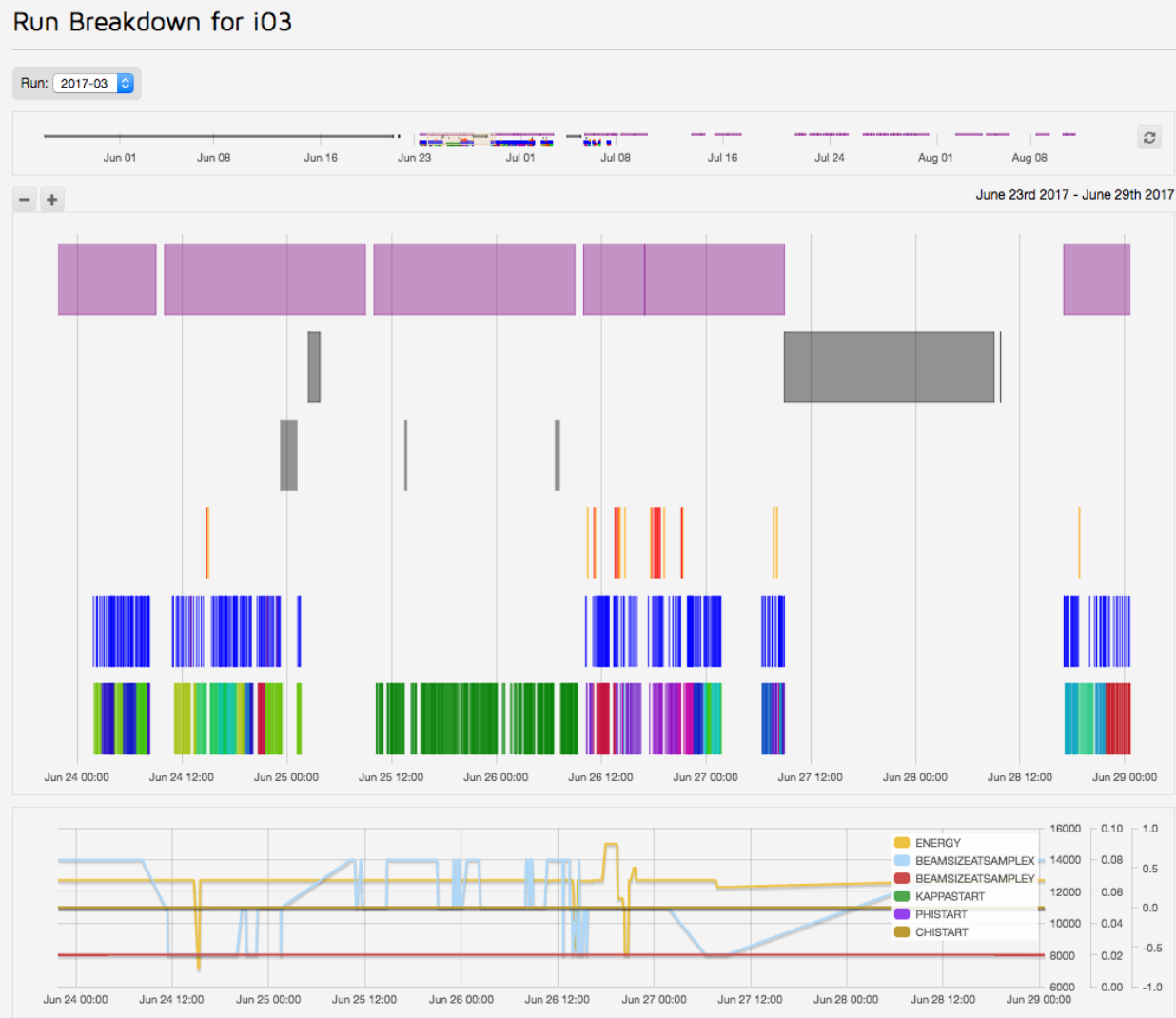- Samples loaded, data collections per hour, etc

Extensive Reporting Statistics

- Beamline parameters histogrammed per run (can plot multiple and vs. other beamlines)
- How are users using the monochromator, slits, mirrors, detector, etc

Extensive Reporting Statistics

- Beamline at a glance per run

Extensive Reporting Statistics

BAG Overview

This page shows BAG overview statistics for the selected time period

Run: 2017-03 ☐ Scheduled Visits Only

Yearly | Monthly | Weekly

mx | sx | nt | in | cm | sp | sw | sm | mt | nr | lb

Search

Proposal	No. Visits	Allocated (hr)	Remaining (hr)	Used (%)	Data Collections / hr	Max / hr	Total	Screenings / hr	Max / hr	Total	Samples Loaded / hr	Max / hr	Total
mx	4	62	0	100	2	4	26	6	19	78	8.6	19	103
mx	4	53	0	100	4.9	7	34	13.7	20	96	14.9	20	104
mx	3	62	0	100	6.2	10	105	5.1	10	87	9.1	14	154
mx	6	131	0.1	99.9	5.4	14	118	7.7	22	169	10.7	24	236
mx	7	115	0.1	99.9	7.4	15	170	13.3	30	307	12.9	30	297
mx	9	88	0.4	99.5	4.8	12	124	5.8	12	151	9.7	19	253
mx	2	39	0.7	98.3	4.3	9	68	7.7	15	123	9	16	144
mx	5	51	1.3	97.5	19.3	28	270	0.3	3	4	18.3	27	274
mx	7	74	2.3	96.9	3.9	13	58	6.5	19	97	7.8	19	125
mx	10	168	5.7	96.6	2.9	14	145	8.1	24	404	9.8	23	478
mx	2	46	2.3	95.1	6.9	30	138	4.4	18	87	9.7	19	193
mx	2	46	2.5	94.6	0.4	3	9	0	0	0	11.3	23	225
mx	9	168	9.9	94.1	3.4	16	151	12.4	22	545	12.4	28	560
mx	1	7	0.4	94	7.3	15	51	0.4	2	3	6.9	18	48
mx	3	39	3.5	91.1	1.5	5	6	0	0	0	5.5	6	11

15 ☐ Page « ‹ 1 2 3 › »

- BAG performance per run
- Allocated and used beamtime, samples, datacollections, etc

VMXi Crystal Screens

Crystallisation Screens

This page lists all available crystallisation screens.

+ Add Screen

Name	Global	# Groups	# Components
HR-Crystal Screen Cryo HT	Yes	96	319
HR-Crystal Screen HT	Yes	96	237
HR-Crystal Screen Lite	Yes	50	121
HR-Detergent Screen 1			
HR-Detergent Screen 2			
HR-Detergent Screen 3			
HR-Detergent Screen HT			
HR-Grid Screen Ammonium Sulfate			
HR-Grid Screen MPD			
HR-Grid Screen PEG 6000			
HR-Grid Screen PEG/LiCl			
HR-Grid Screen Salt HT			
HR-Grid Screen Sodium Chloride			
HR-Grid Screen Sodium Malonate			
HR-Index Screen			

Crystallisation Screen

This page lists details for the selected crystallisation screen.

Name   HR-Crystal Screen HT

Global   Yes

Capacity   96

Screen Components

Component	Concentration		pH
calcium chloride	0.02	M	
sodium acetate	0.1	M	4.6
2-methyl-2,4-pentanediol	30	%(v/v)	

Position

1	2	3	4	5	6	7	8
13	14	15	16	17	18	19	20
25	26	27	28	29	30	31	32
37	38	39	40	41	42	43	44
49	50	51	52	53	54	55	56
61	62	63	64	65	66	67	68
73	74	75	76	77	78	79	80
85	86	87	88	89	90	91	92

- Have database-ised all crystal screens from Australian source data
- Long term means we will be able to trace crystal conditions -> diffraction quality

Electron Microscopy

Data Collections
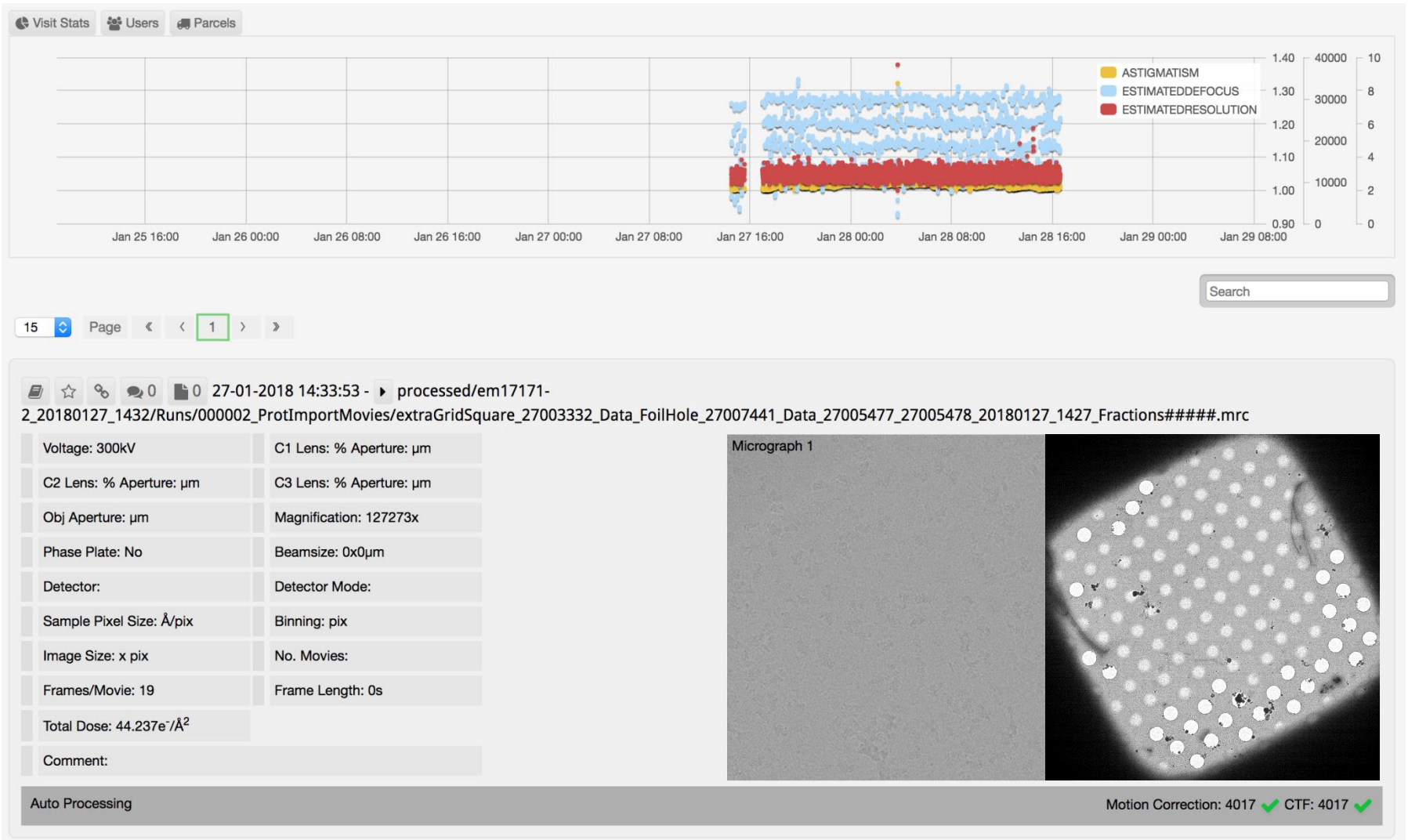
- Currently Atlas = ISPyB Data collection
- Scatter plots show Microscope vitals in real time
- Processing status updated in real time

Processing
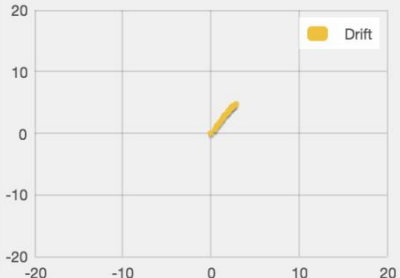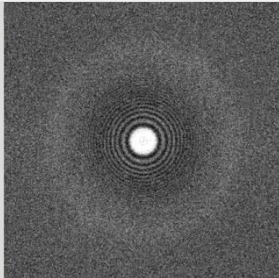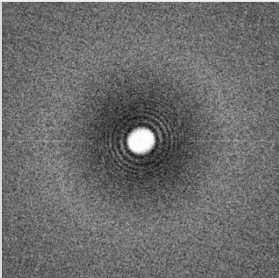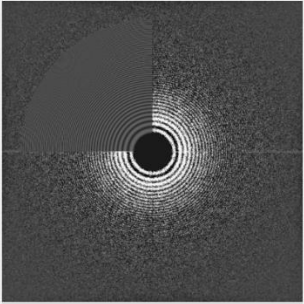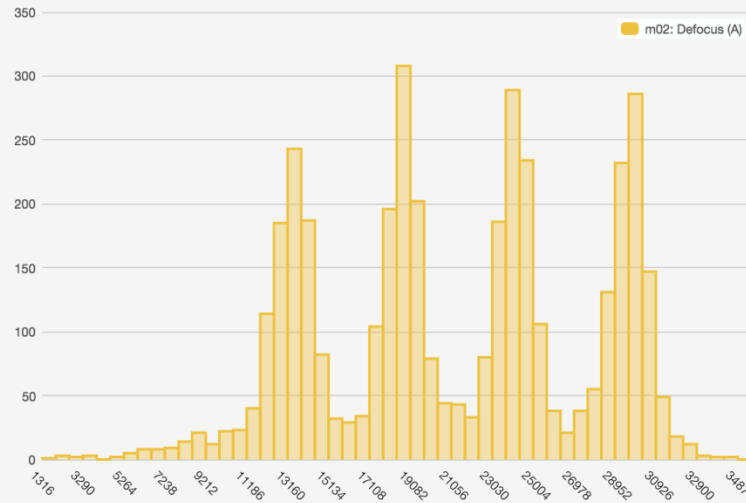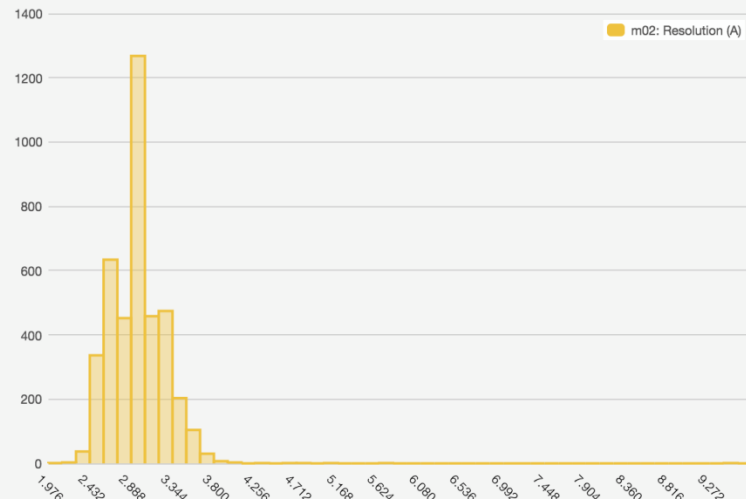

- Have output from Motion Correction & CTF Correction
- Motion Correction: Drift plots, some correction parameters
- CTF: Some parameters, FFT theoretical vs. real
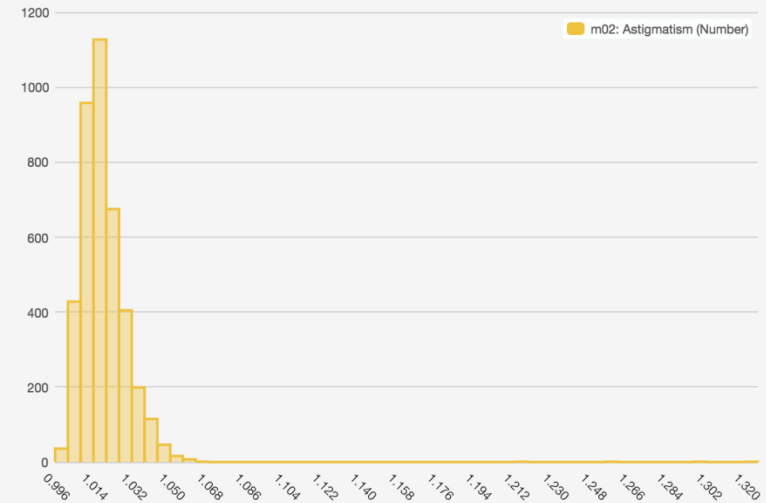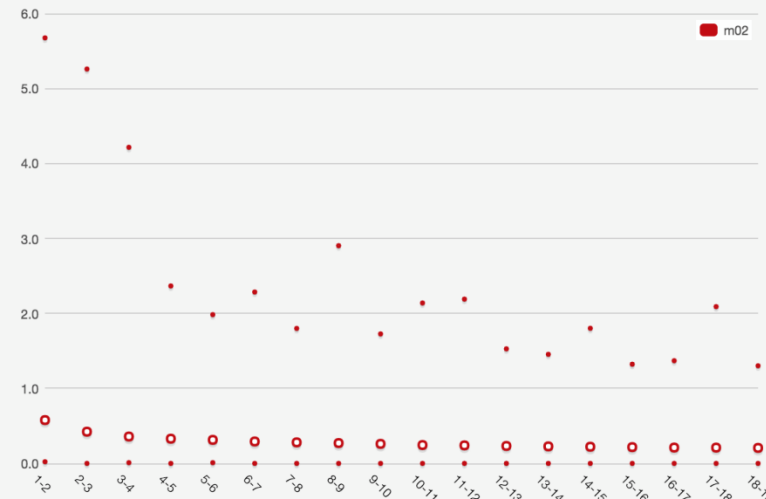
Visit Stats

Histograms

- Usual SynchWeb visit stats (pie chart of time, faults, etc)
- Additionally histograms of microscope vitals

EM Developments

- Would like to:
  - Record Atlas as datacollection group
  - Record one datacollection per GridSquare
  - Heatmap across grid square to show sample quality

- Then have nice hierarchy for exploring data