ISPyB at Diamond

Neil A Smith

ISPyB Meeting 13th September 2018

ISPyB Updates

- System architecture and status
- Feature updates for beamlines
- Developer tools
- Developer meetings

ISPyB at Diamond: System architecture

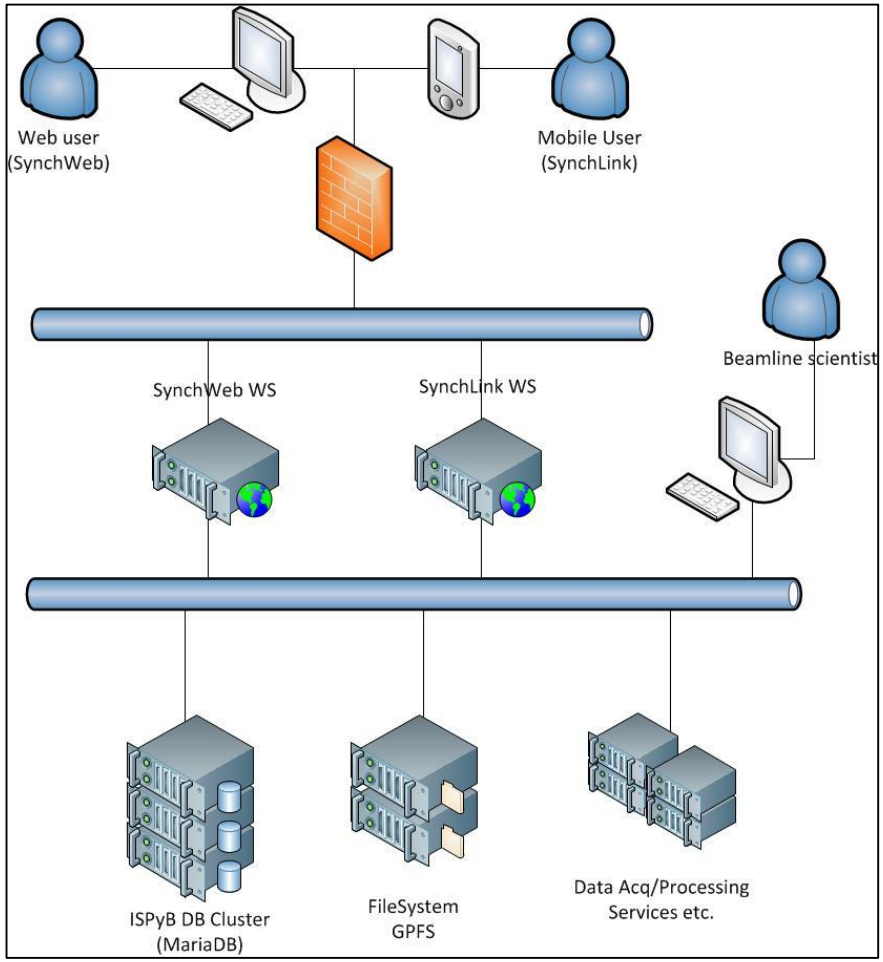
ISPyB database in production

Maria DB (3 nodes) with Maxscale proxy

Main web application and services provided by SynchWeb

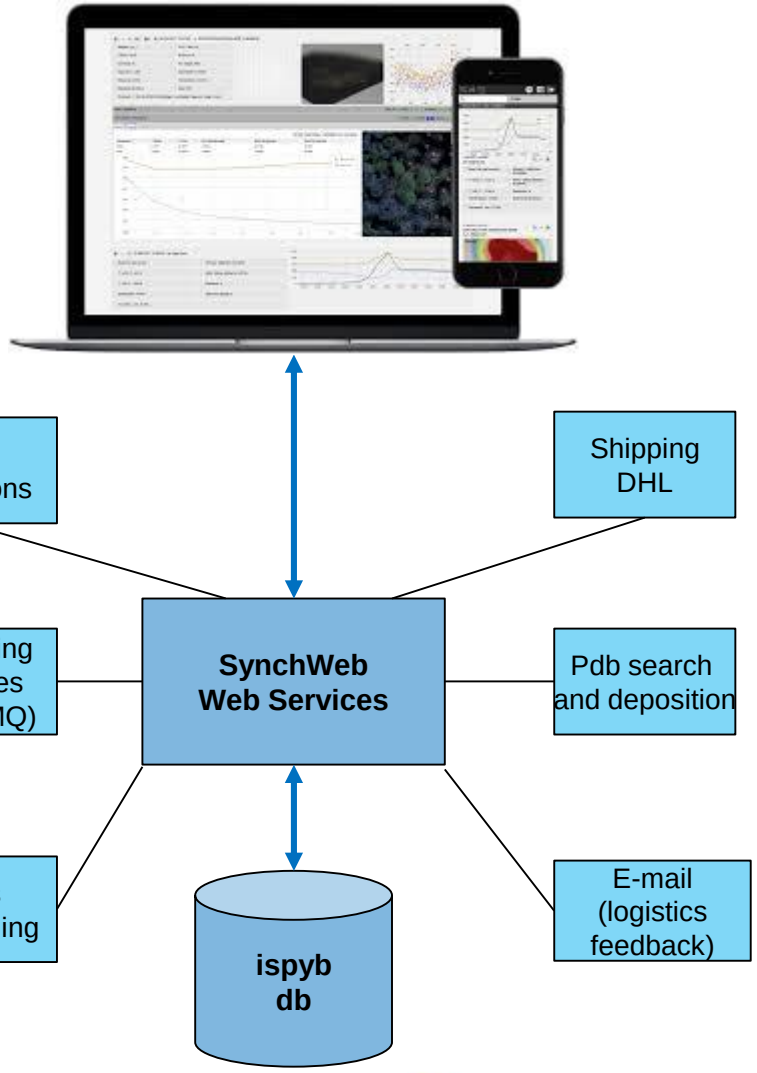
Supported interfaces for clients include python and Java stored procedure API

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



ISPyB at Diamond: SynchWeb

- SynchWeb provides software stack to handle shipping, data collections etc.
- Integrates with Diamond processing pipelines and third party APIs (DHL, PDB etc.)
- All meta data stored in ISPyB database



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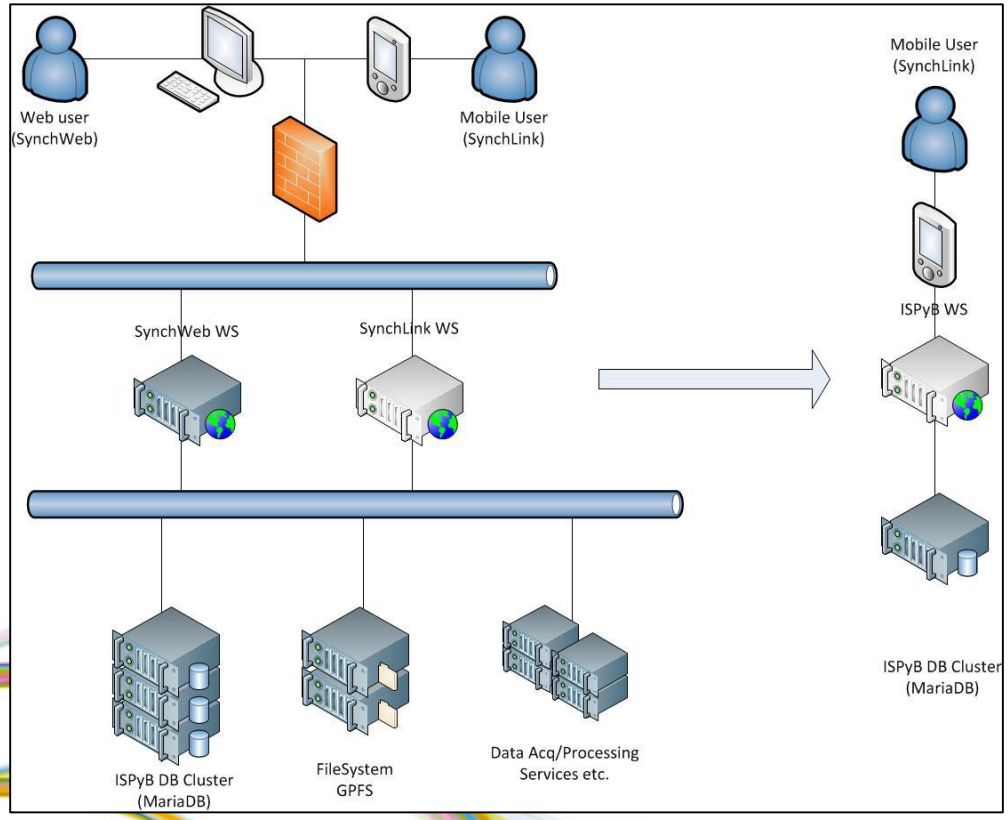
ISPyB at Diamond: Integration of Java Web Services

Migrate bespoke mobile services to ISPyB



Replacing bespoke web services with ISPyB WS

Contractor brought in to develop ISPyB web services for SynchLink (Talk later…)

Also supports remote shipping with University of Oulu

ISPyB Updates: Feature updates for beamlines

MX

- Improved view of auto processing results (i.e. summary table)
- Enhanced Dewar tracking in facility and user e-mail feedback
- Move towards use of registered containers “only”; precursor to increased automation

XPDF

- Improvements to GDA allowing data collections written to ISPyB

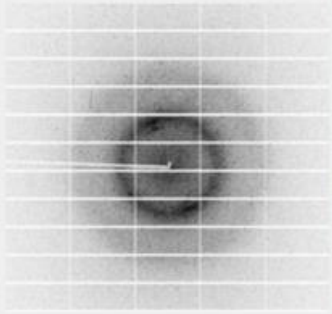
VMXi

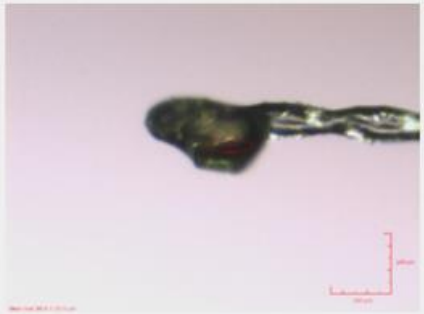
- UI improvements for presenting drop scoring results in plate view
- SynchWeb supports UV imaging as well as visible
- Heat map on plate view for multiple Regions of interest / Points of Interest
- Global presets for beamline setup/data collection parameters for remote operation

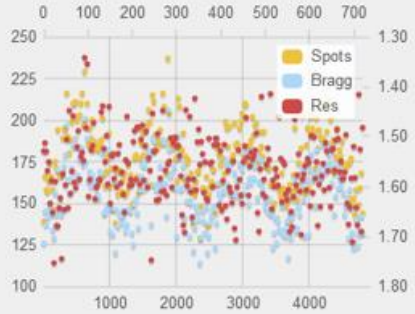
Lots of minor bug fixes and feature improvements…
Lots of new requirements too…

0 1 17-08-2018 13:54:26 - 2018-08-17/test135424/INS2_1_####.cbf

Sample: INS2	Flux: 4.81e+4
Ω Start: 0.0°	Ω Osc: 0.15°
Ω Overlap: 0°	No. Images: 4800
Resolution: 1.41Å	Wavelength: 1.2000Å
Exposure: 0.040s	Transmission: 6.25%
Beamsize: 80x20µm	Type: SAD
Comment: Simulated datacollection.	







Auto Processing — Fast DP: ✔ Xia2: ✔ ✔ MultiXia2: ? ? autoPROC: ✔

Type	Resolution	Spacegroup	Mn<I/sig(i)>	Rmerge Inner	Rmerge Outer	Completeness	Cell
fast_dp	27.60 - 1.45	I 2 3	56.8	0.053	0.814	100.0	78.08 78.08 78.08 90.00 90.00 90.00
xia2 dials	39.04 - 1.27	I 2 3	39.7	0.047	2.104	99.9	78.08 78.08 78.08 90.00 90.00 90.00
xia2 3d	27.60 - 1.31	I 2 3	40.0	0.047	2.221	100.0	78.07 78.07 78.07 90.00 90.00 90.00
xia2 3dii	55.20 - 1.31	I 2 3	40.2	0.046	2.223	100.0	78.07 78.07 78.07 90.00 90.00 90.00
autoPROC	55.21 - 1.30	I 2 3	40.4	0.048	4.849	100.0	78.08 78.08 78.08 90.00 90.00 90.00
autoPROC+STARANISO	55.21 - 1.29	I 2 3	41.3	0.048	3.960	96.6	78.08 78.08 78.08 90.00 90.00 90.00

fast_dp | xia2 dials | xia2 3d | xia2 3dii | autoPROC | autoPROC+STARANISO

Plots | MTZ file | Log file | Archive | Files | Lookup Cell

Beam Centre	X	Y
Start	214.56	210.97
Refined	214.54	211.04
Δ	0.02	-0.07

Space Group	A	B	C	α	β	γ
I 2 3	78.08	78.08	78.08	90.00	90.00	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	73993	1023	1.45 - 1.49	0.825	7.3	1.0	99.8	72.3	99.4	36.6	-0.0
innerShell	12206	178	6.48 - 27.60	0.054	135.8	1.0	98.8	68.6	99.2	40.2	0.6
overall	1098493	14245	1.45 - 27.60	0.057	56.8	1.0	100.0	77.1	99.9	39.4	0.5

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Dewar Tracking

- Rack positions in storage area are barcoded
- Dewar location is recorded by scanning the barcode of the dewar label followed by the rack barcode
- Any rack position can be used, no need to organize by beamline
- Efficient use of storage and easy to find dewars

Dewar Overview

This page shows all dewars for all current visits

i02 i02-2 i03 i04 i04-1 i23 i24

Imager Requested

First Experiment:

Search

Start Date	Visit	Beamline	Local Contact	Shipment	Dewar Name	Dewar Code	Containers	Courier	Track # to	Status	Location	Tracking
09:00 26-10-2018	cm19647-5	i02-2		cm19647-5_Shipment1	cm19647-5_Dewar1					processing		
10:00 04-08-2018	mx18515-3	i04-1		mx18515-2 300418	DLS-MX-0663	DLS-MX-0663	DLS-0022, CPS-1687, DLS-0023, EDI-0003, DLS-0024, EDI-0005	DHL	7981388354	at facility	stores-out	Delivery: OXFORD-GBR
10:00 16-07-2018	in20016-5	i24		Swe AZ 180521 dewar2	BackupDisk			Fedex		opened		
10:00 07-07-2018	mx15806-17	i04		DREW-SU-mx15806-16	Dewar1		CPS-2799, CPS-2614, CPS-2612, cps-2615, CPS-2613, CPS-2617, CPS-2618	YSDS		at DLS	RACK-X2	
10:00 06-07-2018	mx19458-2	i24		vmxi_plates_juan	Dewar1		pbp5_vmxitest, pbp5_vmxi_test2, pbp5_plate2	banana		opened		
09:00 20-06-2018	nr19737-3	i03		nr19737-3_Shipment1	nr19737-3_Dewar1					at DLS		
10:00 22-05-2018	mx15916-58	i04	Dr Dave Hall	180522_I04_Graham	Graham	DLS-MX-0628	CPS-2310, CPS-2311	DHL		at facility	stores-out	
10:00 22-05-2018	mx15916-58	i04	Dr Dave Hall	180522_I04_Graham	Deane-I04	DLS-MX-0629	CPS-2319, CPS-2317, CPS-2320, CPS-2322, CPS-2321, CPS-2318, CPS-2316	DHL		at facility	stores-out	
10:00 22-05-2018	mx15916-58	i04	Dr Dave Hall	YAN_i04_MX15916-58	DLS-MX-0481	DLS-MX-0481	CPS2278, CPS2280, CPS2279	DHL	4173444015	at DLS	RACK-C3	Delivery: OXFORD-GBR
10:00 22-05-2018	mx15916-58	i04	Dr Dave Hall	mx15916-58_Shipment1	mx15916-58_Dewar1	DLS-MX-0618	DLS-0097, DLS-0092, DLS-0092, DLS-0094, DLS-0098	Cambridge Courier		at facility	stores-out	
10:00 22-	mx15916-	i04	Dr Dave Hall	MRC_LMB_Mark	DLS-MX-	DLS-MX-	LMB-007	DHL	2513853845	at facility	stores-	Delivery: OXFORD-GBR

ISPyB Development tools

- Virtual environment setup for new developers
- Creates set of VM using Vagrant and Ansible
- Provides full LAMP stack (Linux, Apache, MySQL and PHP)
- Checkouts and build SynchWeb code
- Also provide option for integration with Central Authentication Service (CAS)

https://github.com/drnasmith/synchweb-devel-env

- Similar version created for Java ISPyB web services
- Requires some manual steps currently (deploying ISPyB ear file)

https://github.com/drnasmith/ispyb-devel-env

- Also created a simple web based ISPyB admin tool

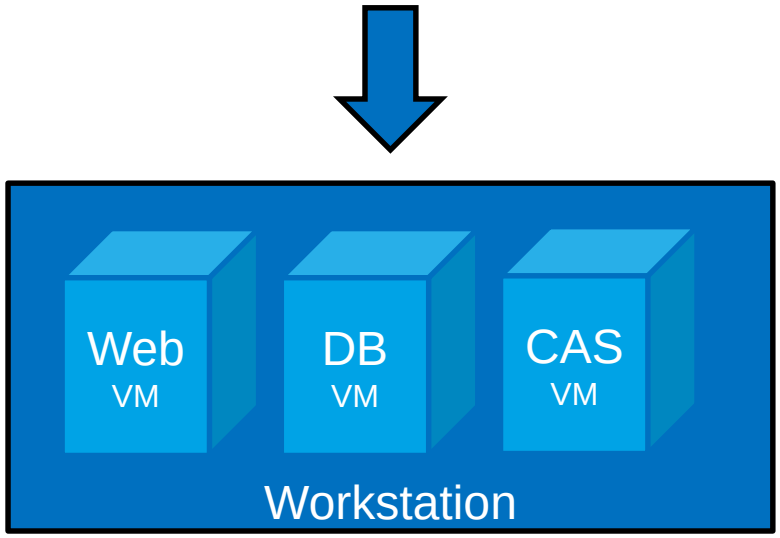
https://github.com/drnasmith/flask-ispyb-admin

build_synchweb.yml

```
# This playbook downloads and builds SynchWeb on a local filesystem.
# It will build a copy for each host listed in inventory files and is a prepa
# Its good practice to use different host files for staging/development and p
# This playbook makes use of "local_action" so it runs for each host but buil
# Build output is stored in ((synchweb_build_dir)) e.g. software/cs04r-sc-vse
- hosts: all

  name: Checkout and build the SynchWeb code
  tasks:
  # Checkout latest git from master
  - name: Checkout SynchWeb code from github
    local_action:
      module: git
      repo: https://github.com/DiamondLightSource/SynchWeb.git
      dest: "{{synchweb_build_dir}}"
      version: "{{synchweb_version}}"

```



ISPyB: Developer meetings

- Since last face to face meeting we have held monthly video conferences

- Meta data for plates
- Discussed process for agreeing database changes
- Data model documentation
- Anisotropic diffraction parameters
- Closed numerous database issues

- Regular participation from DLS, ESRF, EMBL and Global Phasing
- Others welcome!