Status update

Diamond Light Source

30 June 2020

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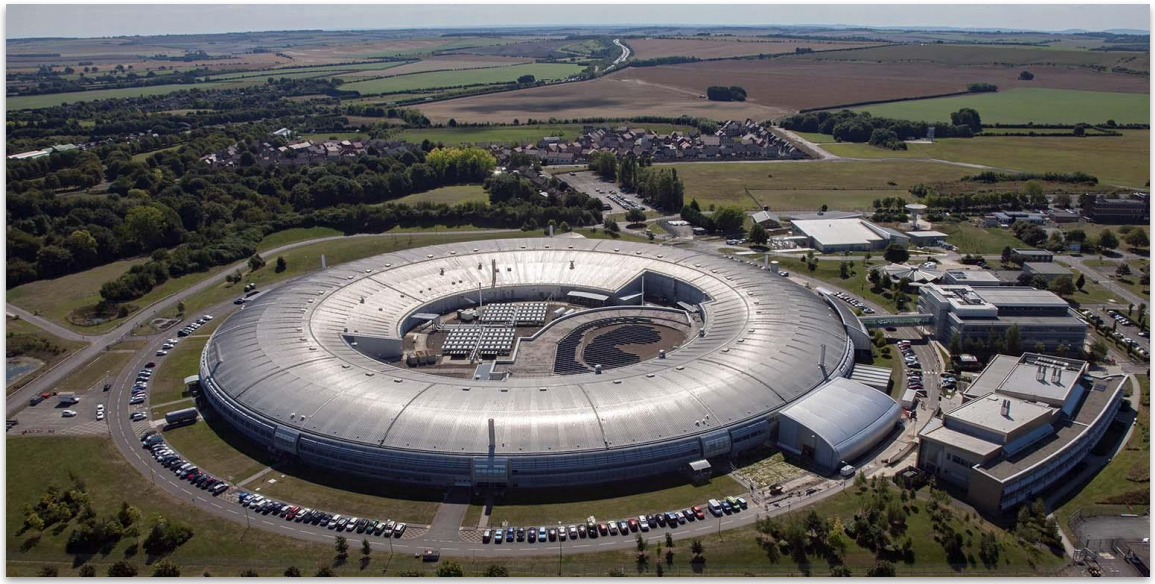
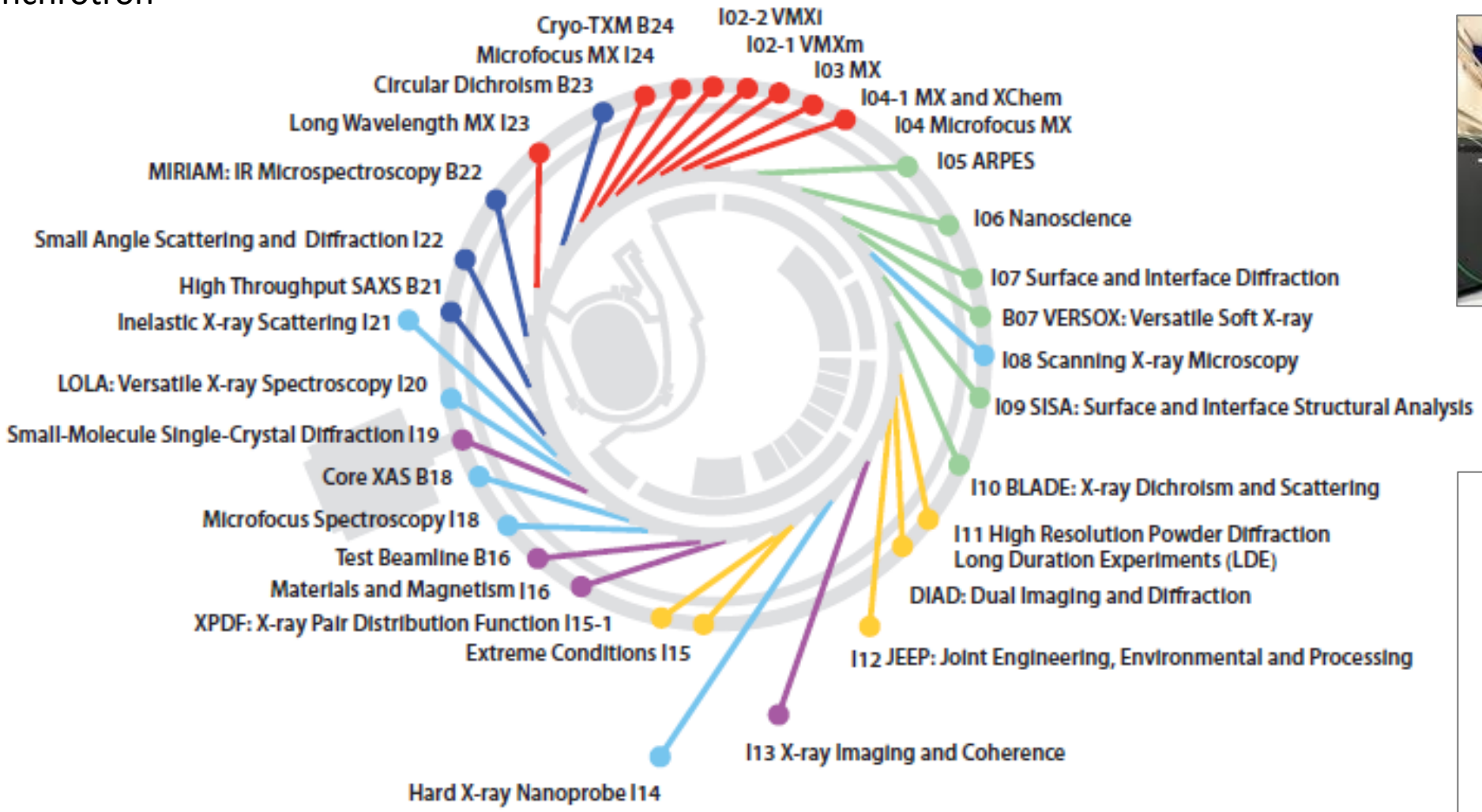


Diamond Light Source, Didcot, UK

Facility Overview

MX | Cryo-Imaging | Soft Cond. Matter | Crystallography | Magnetic Materials | Spectroscopy | Surfaces & structures | Imaging and Microscopy

Synchrotron



Electron Bio-Imaging Centre (eBIC)

~5000 hours beamtime per year
~9000 visits/sessions per year
30 Operational Beamlines
6 Operational EMs
Producing up to ~60TB per day
Currently 25PB in archive, 6PB last year
Univa Grid Engine based HPC (~6,500 CPU cores, ~240 GPUs)
GPFS for storage

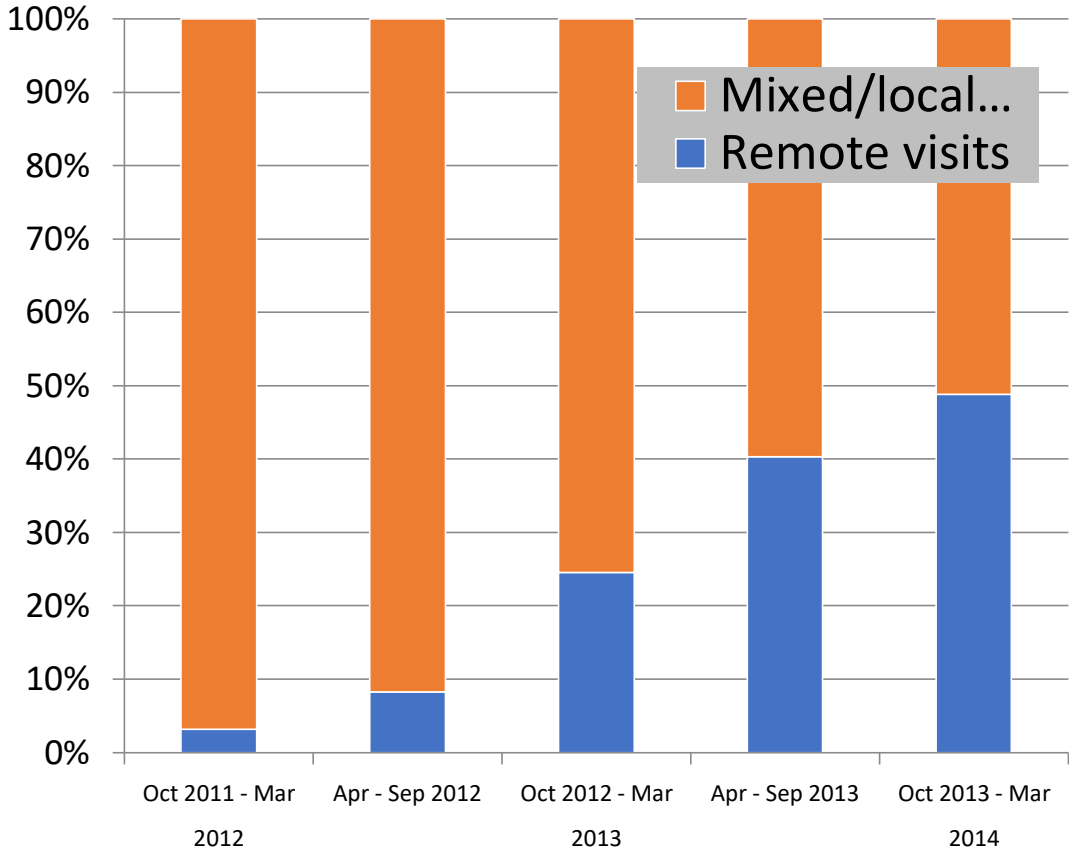
Remote operation

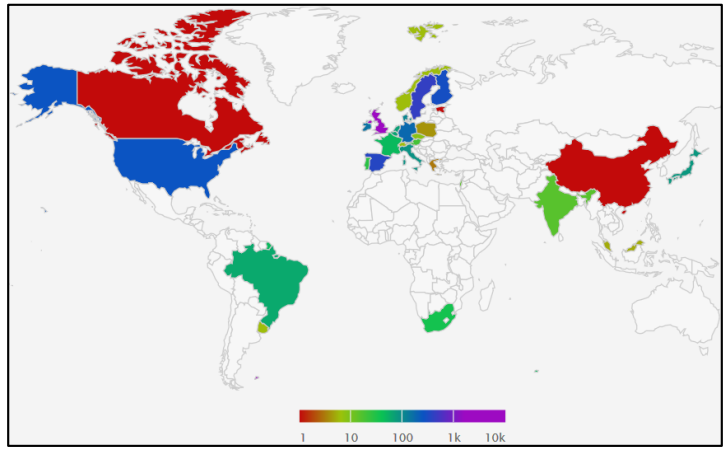
Initial Operation

- Lockdown in UK started 23rd March 2020
- Machine back up from Friday 27th March to Tuesday 3rd April for commissioning
- User operation for COVID research only from 31st March running a Tuesday – Friday pattern
  - Opening up to other remote research in June
- A subset of beamlines from I03, I04, I04-1, I24, B21, B23, B24 in use each period (limiting staff on site)
- eBIC operated up to two Titan Krios microscopes running Monday to Fridays
- 3D print farm established supporting local initiative to provide PPE

MX Operation

- Trend towards remote operation apparent before COVID
- Significant usage completely remote
  - 2015 ~50% Remote, 20% mixed, 30% on-site
  - 2018 70% visits to I03 and I04 fully remote
  - 2019 75-80% sessions on I03, I04, I04-1 and I24 remote or automated
- Shipping handled through SynchWeb and ISPyB with DHL integration
- Unattended Data Collection (UDC) recipes selected when creating shipment
- Some of heaviest remote users as close as Oxford and London

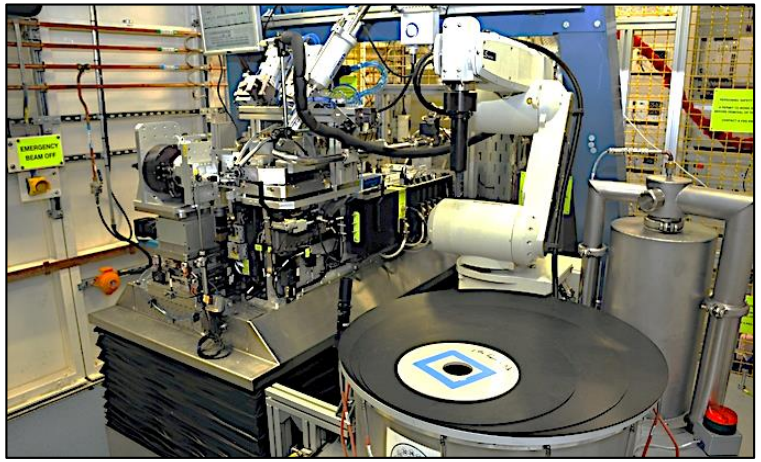


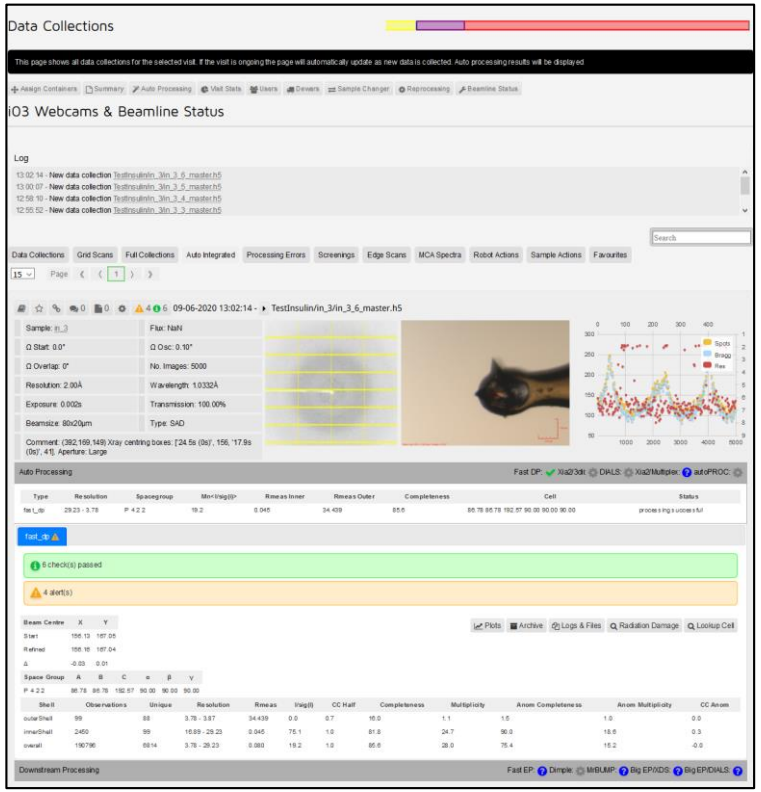


Dewar stats per country

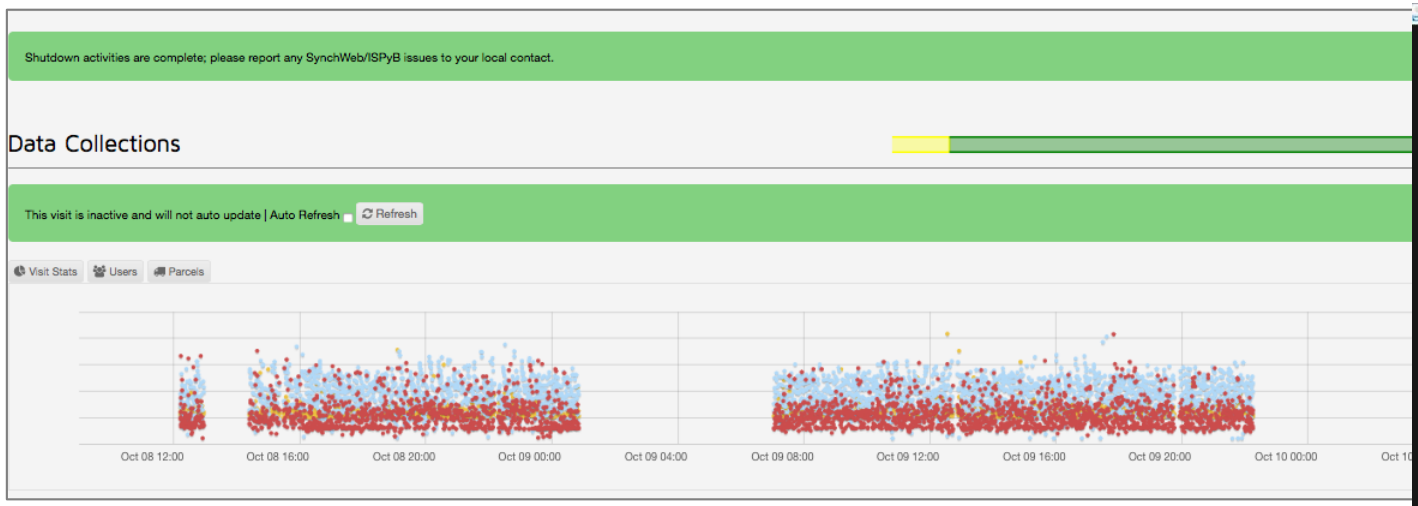
MX Support

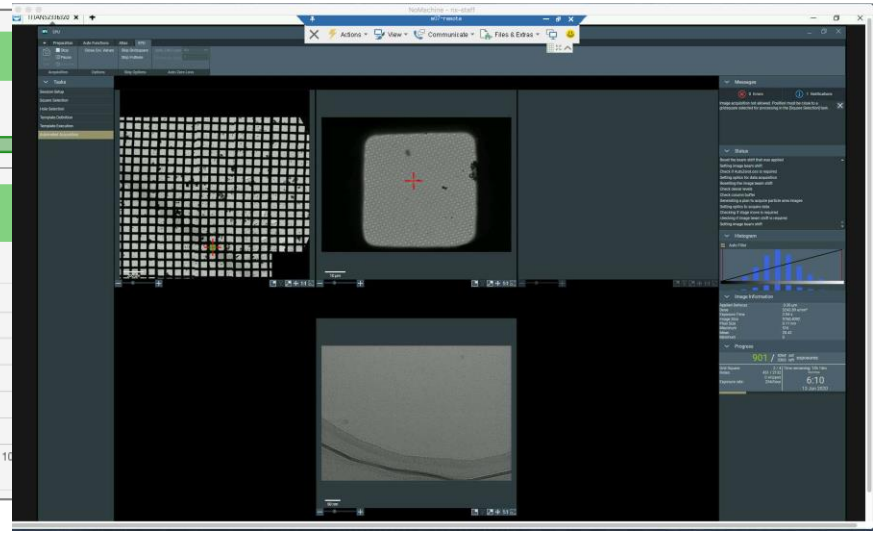
- Beamline staff load sample changer with pucks, perform beamline checks
- During a remote session users connect via NX (NoMachine) to access GDA
- Local contact support available via phone
- Recently LCs have been using Zoom to help provide support during lockdown
- Results reviewed by users via SynchWeb/ISPyB

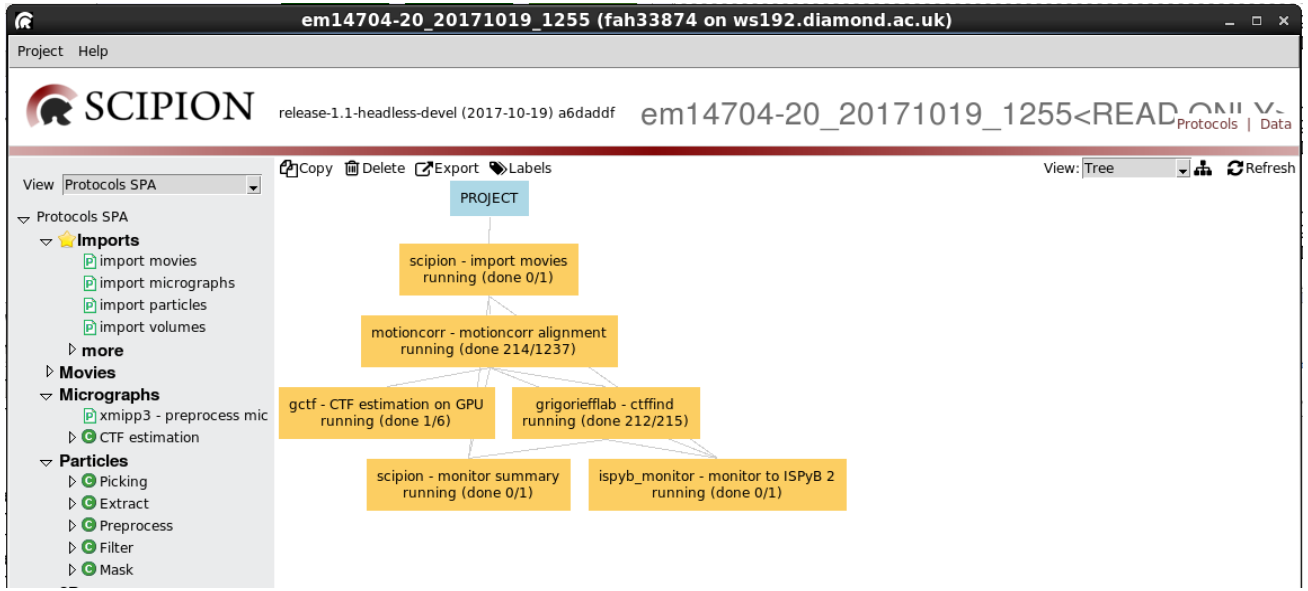




eBIC Operation







- Access to microscope control via NX and TeamViewer, monitored by staff
- Work ongoing to support Relion processing to replace Scipion before lockdown
- New appointment of Senior Software Scientist for EM data analysis

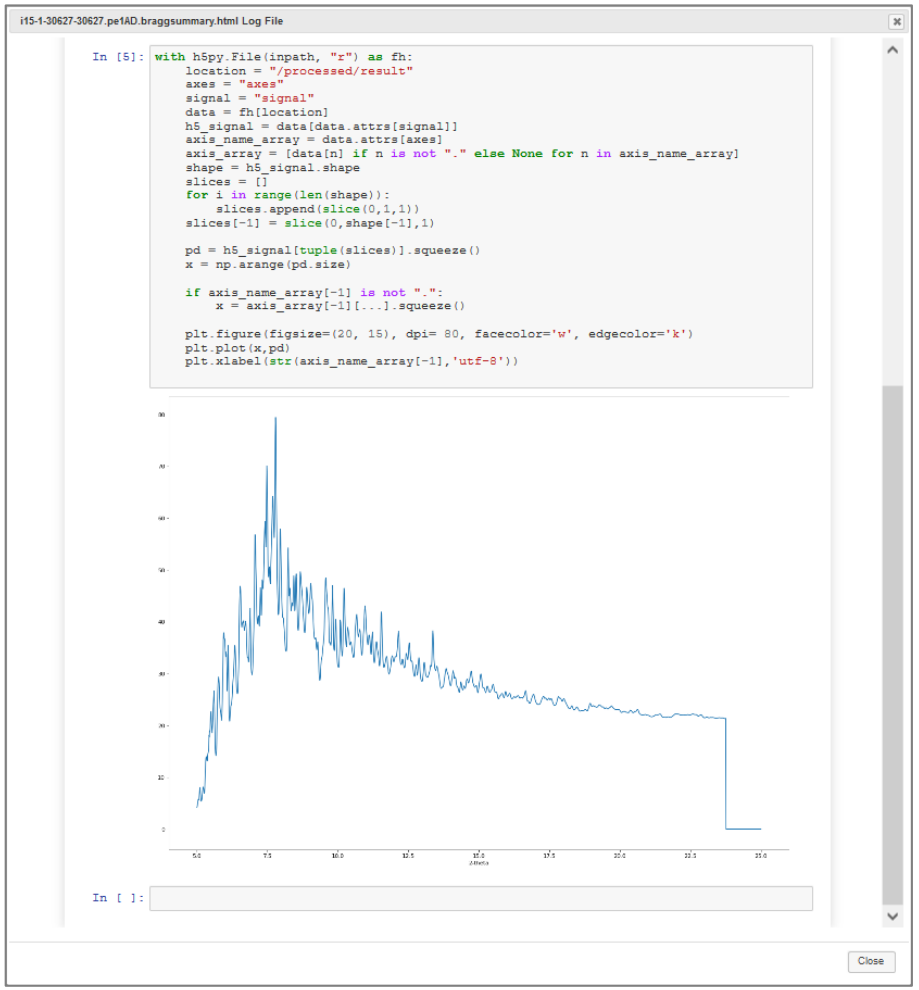
Software developments

- Main focus on making the interface between User Administration System (UAS) and ISPyB robust for UDC
  - Includes better propagation of changes in UAS sample information with ISPyB
  - Enforcing use of approved samples earlier in the process
- Supporting a “responsive remote” scheduling type
  - Easier way to send samples to site without a scheduled session or UDC
- Capture user preference for priority processing at shipment stage
  - Method to manage cluster compute resources if required
- SynchWeb modernisation
  - Research moving from “Marionette with Vue” to “Vue with Marionette”

Future plans

Increased emphasis on remote operation and mail-in for samples

- Project in early stages to allow shipment/mail-in through for Soft Condensed Matter (SCM) group
- Expand use of mail-in for Crystallography group
  - i19 beamlines already using MX capability,
  - i15-1 XPDF work on going – new robot plus JupyterHub for analysis
- Main challenge is extending ISPyB schema to support non-MX sample descriptions



Summary

- In general existing remote capability has worked during lockdown
  - Already well provisioned with NX capability but increased memory usage per server to cope with increased demand
  - VPN upgrades in progress
- Impact on data analysis software engineers manageable via ssh/NX to workstations or via VPN
- More impact on controls software engineers due to limited access to lab based hardware
  - Also callouts / trouble shooting more difficult off-site
- Remote operation has increased in priority so might also lead to more developer resources

Questions?