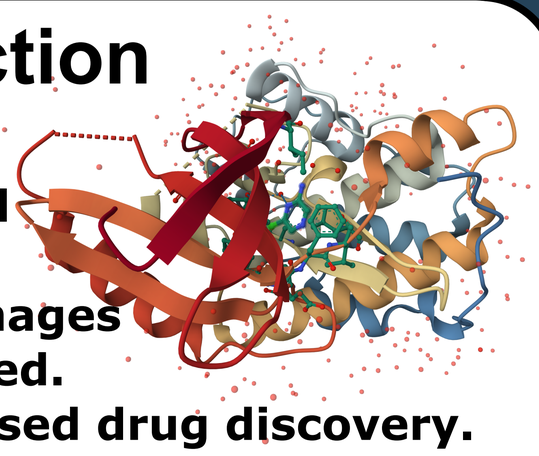
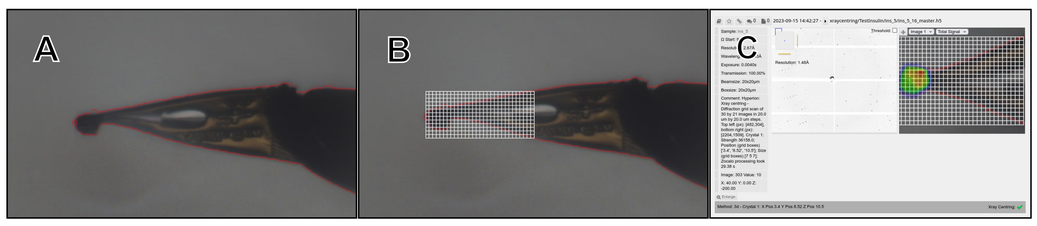
Ultra-high Throughput Macromolecular Crystallography Data Collection Using the Bluesky Framework

D. Perl, N. Frisina, D. Oram, N. Paterson,
Diamond Light Source, Didcot, UK

MX data collection



- Align a protein crystal with the X-ray beam.
- Capture diffraction images as the crystal is rotated.
- Used for fragment-based drug discovery.
- Completely automated at some beamlines.



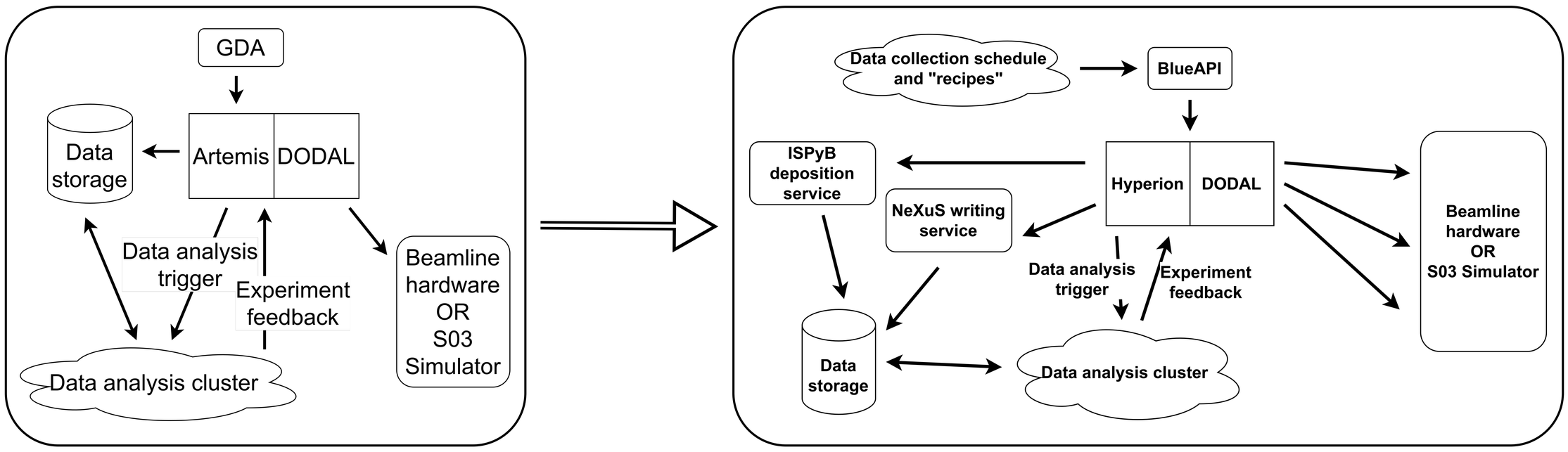
Bluesky[1]

- Modern Python library for experiment control.
- Developed at NSLS-II, in collaboration with other facilities including DLS.
- Good separation of harware interaction and data management.
- Easy integration with other scientific Python libraries.

bluesky

Hyperion

- Application for unattended data collection, built with Bluesky.
- Uses DODAL, a library to contain and organise all hardware at DLS.
- Part of the new DLS Athena[2] platform to support Diamond-II.
- Step-by-step replacement of routines in the legacy data acquisition software.
- Modular design follows naturally from the way Bluesky works.
- Well tested against beamline simulations.
- Currently in transition from prototype to full version.



References

[1] D. Allan, T. Caswell, S. Campbell, and M. Rakitin, ‘Bluesky’s Ahead: A Multi-Facility Collaboration for an a la Carte Software Project for Data Acquisition and Management’, Synchrotron Radiat. News, vol. 32, no. 3, pp. 19–22, May 2019, doi: 10.1080/08940886.2019.1608121.

[2] J. Shannon, C. Forrester, and K. Ralphs, ‘Diamond Light Source Athena Platform’, presented at the ICALEPCS’23, Cape Town, South Africa. Paper TH1BCO05

Faster data acquision

- A fragment screening experiment takes hundreds or thousands of datasets.
- Hyperion will support new kinds of experiments allowing thousands of data collections per day.
- Initial prototype for centring has already increased throughput from ~380 to ~500 samples per day.