Artemis: 3D Gridscans in Bluesky

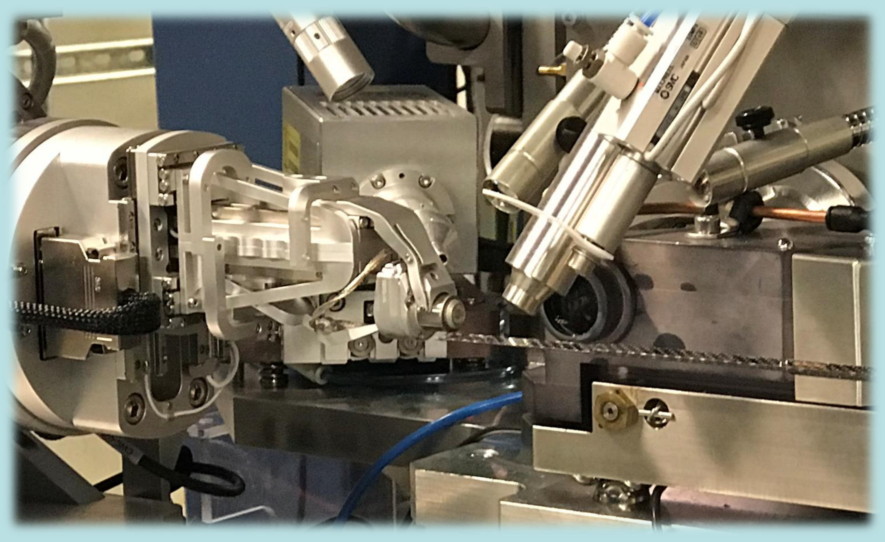
Dominic Oram, Abigail Emery, Helen Forrest, Benjamin Taylor, Matthew Pritchard

Gridscans at Diamond's I03 Beamline

I03 is a macromolecular crystallography (MX) beamline located at the Diamond Light Source (DLS) in the UK. Since 2020 it has been running almost entirely in an automated fashion. Users send samples to DLS and, after the container has been moved to the beamline, they will be analysed with little to no input from staff or users. In this way the beamline can collect high quality data from about 500 samples a day automatically.

I03's sample changing robot is critical to its fast throughput

To allow this automated collection the sample must be centred such that the point which gives the best quality data stays in the beam throughout a rotation scan. Samples are mounted on pins ranging from 100-1000µm, the beam size usually used on I03 is 20x20µm. To provide the best centre the sample is first imaged with an optical camera and positioned such that the tip of the pin is near the centre of rotation, the size of the pin is also determined using this. The beam is then scanned in a grid over the whole sample with short exposures. The data collected at each location is analysed to find the point that provides the most Bragg peaks, which is then used for a full data collection. This 2D scan must be done twice to find the 3D point of interest.



I03's sample area. The Smargon goniometer on the left performs the motion for the 3D gridscan

Given how heavily automated I03 already is there is a great opportunity to provide higher throughput by optimising the time taken for each sample. The gridscan centring is something that must be done for each sample and is currently performed in a suboptimal order so it is a good candidate for performance improvements. This is the aim of the Artemis project.

Artemis vs GDA Gridscan

In total Artemis is expected to take around 25 seconds per 3D gridscan whereas GDA currently takes 50 seconds. Artemis saves time over GDA in a few ways:

1. Both optical images (at 0° and 90°) can be taken immediately after one another. This avoids having to re-configure the beamline for optical/xray collections twice
2. A second optimisation comes from moving more of the logic to the motion controller. In GDA, the motion controller does the 2D gridscan only. In Artemis the controller does the first grid scan, rotation and second gridscan.
3. Lastly, some parts of these steps can be done in parallel. Performing parallel actions on hardware is a lot easier in Bluesky than it is in GDA

This can be illustrated by comparing the order of operations:

Order of Operations	GDA	Artemis
1	Setup for optical image	Setup for optical image
2	Take optical image	Take 2 optical images (90° rotation between)
3	Setup for x-ray data	Setup for x-ray data
4	Trigger motion controller (2D grid)	Trigger motion controller (2x2D grid)
5	Get results	Get results
6	Move to best position	Move to best position
7	Rotate 90°	
8	Repeat 1-6	

Future Plans

- Further testing to improve Artemis accuracy compared to the GDA
- Analyse and improve the performance of Artemis
- Roll out Artemis to other DLS beamlines
- Look for more Bluesky applications across the MX beamlines
- Integrate with the new service architecture being developed for other beamlines around DLS

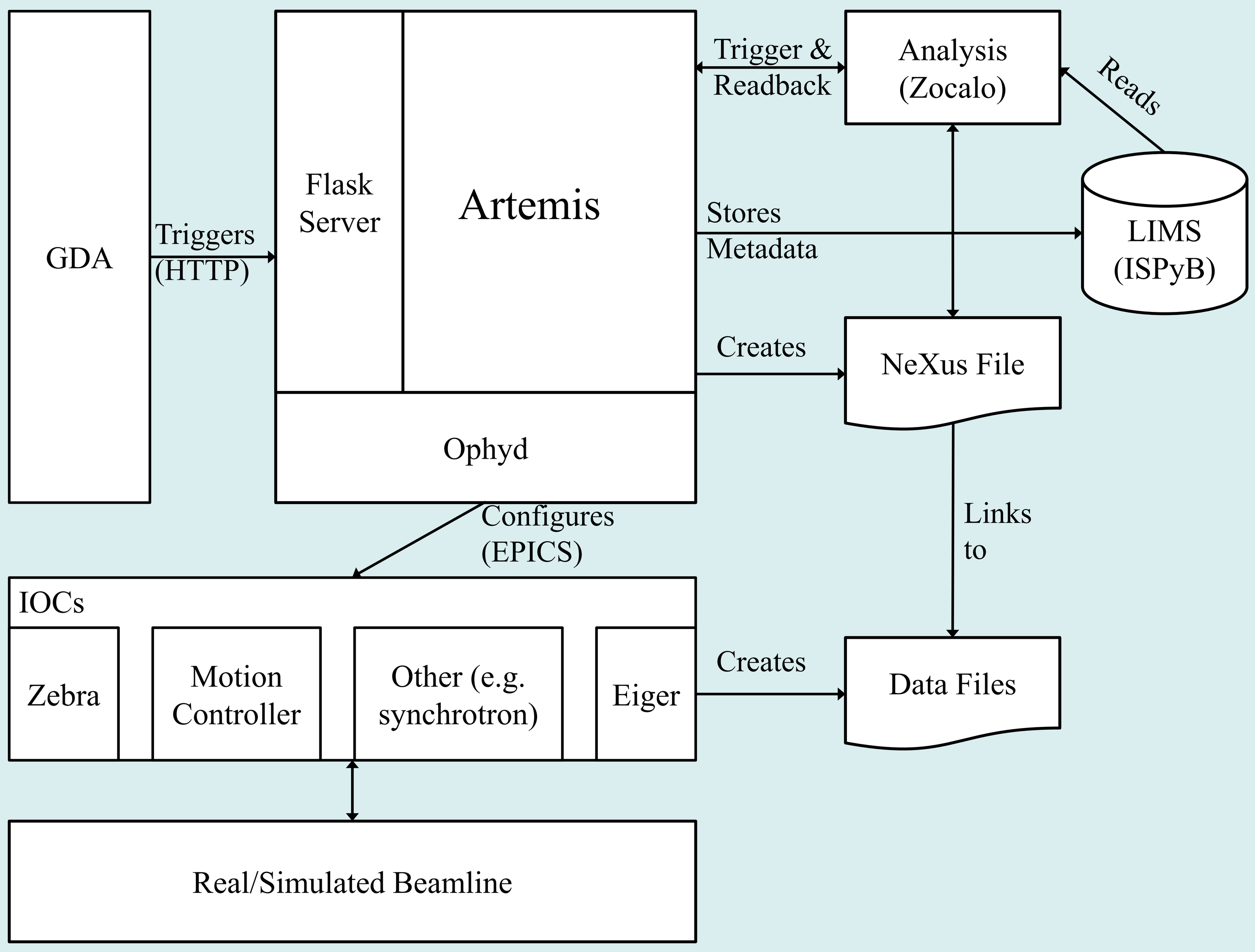
Bluesky at Diamond

DLS will soon be going through a major synchrotron upgrade, Diamond-II. As part of this upgrade several new flagship beamlines have been proposed to make use of the increased flux. The current software stack used for data acquisition, GDA, is quite a complex, monolithic program and has been in use for most of the lifespan of Diamond. As such this hardware upgrade provides an opportunity to also improve the software architecture for the new, and existing, beamlines.

The Bluesky collaboration has been chosen as the basis for this upgrade. The framework was written at NSLS-II and is written in Python 3. Bluesky already provides good support for communicating with EPICS (the control system used at DLS) and for creating and managing scans.

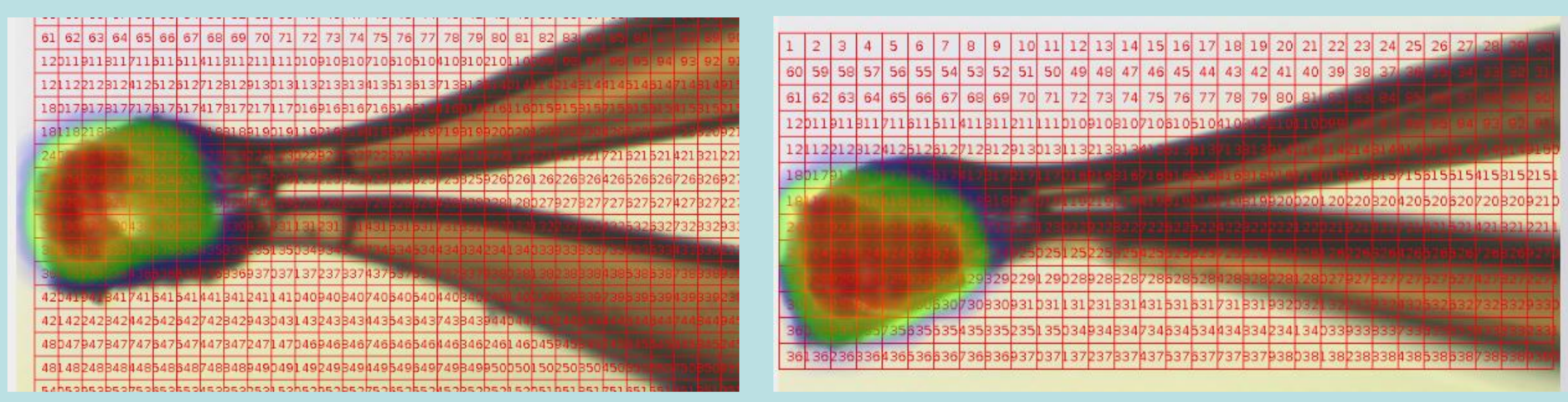
The Artemis project was an ideal candidate for a prototype use of Bluesky at DLS as:

- Adding the faster gridscan into GDA would be complex. This functionality is a core part of GDA and modifying behavior for I03 without negatively affecting other beamlines would be tricky.
- The gridscan is a self-contained. Once it has been performed and Artemis has moved to the centre control can be handed back to GDA for continued data collection
- The project allows us to use better software development practices. GDA has very low test coverage and relies heavily on hardware being available to allow testing. In building Artemis we maintained >85% test coverage and built simulated hardware alongside it allowing for easy offline development.
- The use case requires integration with many existing DLS systems, including being triggered from GDA itself. This proves that we can write plans in Bluesky that create correctly formatted NeXus files, stores data in the LIMS and interacts with the data analysis pipelines



Latest Results

Artemis has been successfully run against user samples on I03. The software stack took data, interacted with DLS infrastructure and moved to the centre as provided by analysis. However, further testing is required to confirm that the centre position returned is correct as it differs from that returned by GDA for the same samples. When performing the gridscan, Artemis is faster than GDA and in some cases nears the 25s target. However, the timing is varied and is not consistent as expected, further profiling is required to find out why.



The two 2D gridscans performed by Artemis. At 0° (left) and 90° (right). The red boxes show each data collection, superimposed on the optical image of the sample. The heatmap shows the results returned from analysis for each collection.

For more information please contact dominic.oram@diamond.ac.uk