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Software Mapping Project with Nanopositioning Capabilities

MARK BASHAM, JACOB FILIK, TOM COBB, JAMES J. MUDD, J. FREDERICK W. MOSSELMANS, PAVEL DUDIN, AARON D. PARSONS, PAUL D. QUINN, AND ANDREW J. DENT
Diamond Light Source, Oxfordshire, UK

Introduction

Diamond Light Source is the UK's national synchrotron facility, entering user operation in 2007 with seven beamlines. With 33 operational beamlines, it has delivered user operations for over 10 years. During this time, Diamond has had to adapt its model of delivering software and hardware solutions to the rapidly expanding number of beamlines. Bespoke per-beamline solutions were possible with the initial seven beamlines, but as the number of beamlines grew, this has been harder to sustain.

In 2014, Diamond decided to provide a unified software and hardware solution to several new and existing beamlines [1], in order to reduce the overall cost of ownership of these systems. By pooling the resources, a software and hardware stack which was highly capable was developed. These beamlines were primarily engaged in mapping X-ray probe experiments, but with differences in detectors, micro- or nanopositioning stage requirements and, ultimately, the science case.

Mapping, or scanning-probe, beamlines conduct a usually rapid series of identical experiments, where the only variable is the spatial position of the X-ray micro- or nanoprobe relative to the sample. Typically at synchrotrons, this involves moving the sample and not the beam, and the pattern traversed by the sample is dependent on the experiment being conducted, but is often an alternating direction raster scan, or snake scan.

Project components

Mapping a sample with high levels of speed, precision, and efficiency is challenging technologically. The nanoscale precision required for modern nanoprobe beamlines presents significant additional challenges. Approaching this with a generic and universal solution which can be easily adopted by any beamline requires a truly cross-disciplinary team and technology stack, ranging from low-level controls through data acquisition and data analysis. For the map-

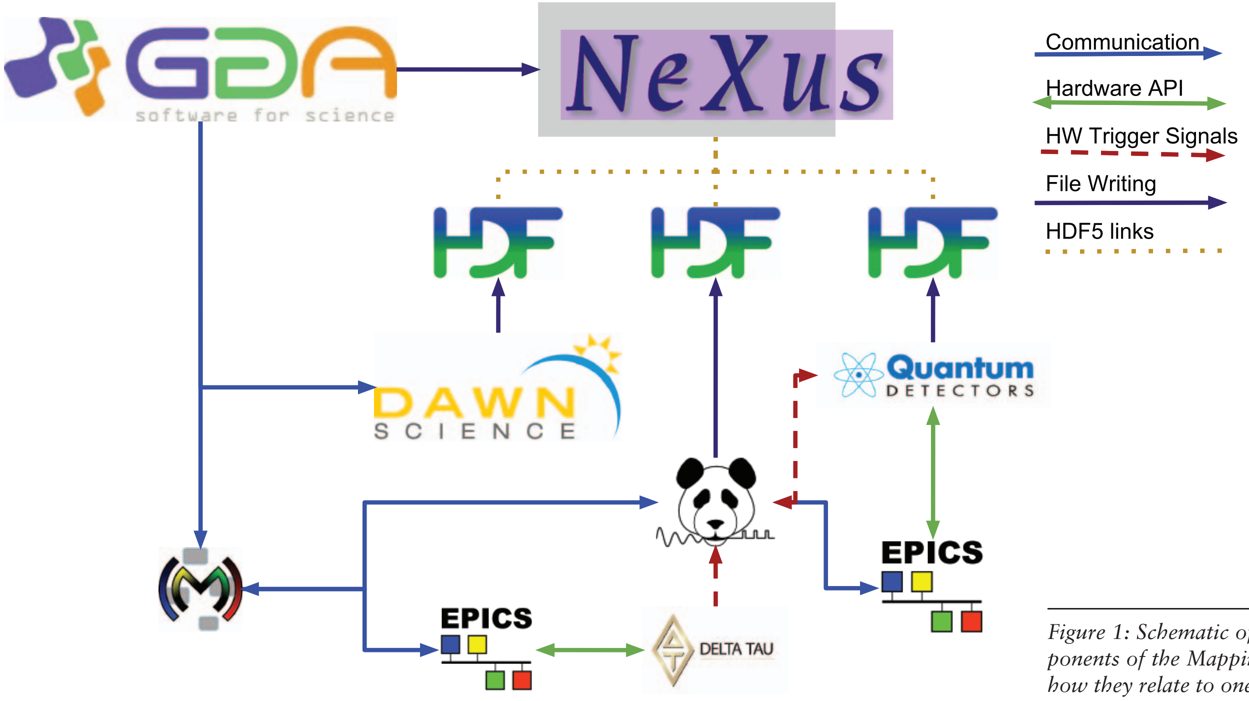


Figure 1: Schematic of the core components of the Mapping Project, and how they relate to one another.

ping project, the following technologies and software solutions were chosen or developed.

HDF5 SWMR (single-writer/multiple-reader)

One of the primary science drivers for the mapping project is to visualize data in many ways during collection. Solutions considered at the start of the project included storing data in memory and live streaming, but none allowed for the full set of features desired by the project. The choice quickly focused on one of the new features of HDF5 being developed by the HDF group but specified and funded by Diamond, ESRF, and Dectris: SWMR [2, 3]. SWMR (single-writer/multiple-reader) mode in HDF5 removes the limitation of vanilla HDF5, which means that the file needs to be closed by the writing process in order to be read by any other process. SWMR, enabled on a POSIX-compliant network file system, such as Lustre or GPFS, allows any number of processes to open the file, refresh it and read the current state as needed.

Using SWMR enables the data being written from the detector to be read and visualized in the data acquisition system, allowing for interactive, real-time feedback to the user. The data can also be read by processing tools, running on HPC to fully analyze the data, writing the processed data to another SWMR file. This, in turn, allows the processed data to be visualized in real time in the data acquisition system.

NeXus

After deciding to use SWMR HDF5 files as the main form of transferring live information about the collected data, it was critical to make sure that the information was written in such a way as to allow visualization and auto processing. To achieve this, the NeXus format [4] was chosen, as it is the adopted standard at many synchrotrons. In recent years, the descriptions of axes and associated metadata have been improved dramatically when dealing with high-dimensional datasets, such as those which are intended to be collected [5].

EPICS

Diamond uses EPICS (Experimental Physics and Industrial Control System) [6] to automate the running of the main particle accelerator, and also for hardware control of most of the beamline systems. EPICS is very good for many control areas, such as motor or temperature control, but it lacks functionality in a few key areas that would let us run high-data-rate hardware-triggered scans. This project involved developing several new pieces of EPICS support, including significant improvements to the Area Detector HDF writer. This allowed SWMR integration, the writing of frames into arbitrary positions in the file, and a plugin to support pausing and rewinding scans. We also improved support for the Delta Tau Geo Brick motion controllers, which are now standard hardware at Diamond, allowing for a series of data points to be streamed onto the controller, and a coordinated series of PVT (position, velocity, time) moves to be performed across a number of axes. The Geo Brick makes sure that the moves are completed within a specified amount of time, and can be run as either a continuous scan or a hardware step and dwell scan. At each preset point in the scan, the Geo Brick outputs a trigger pulse which can be used to synchronize other devices as required. For a scan of two axes on the Geo Brick, a speed of 300 Hz can be achieved with every point in the scan having a uniquely defined position.

Stages

All of the beamlines mentioned use the Delta Tau Geo Brick IMS II for motion control. This flexible motor controller allows PVT trajectory scans of a variety of motors and can read both incremental and absolute encoders for feedback. The micropositioning beamlines can employ an X-Y stack of conventional stepper and servo motors with encoder resolution in the 0.1 um range. The nanopositioning beamlines use the same type of motors in their coarse stages, but place an X-Y piezo actuator stack on top, typically reading the combined motion with an interferometer with picometer resolution. The piezo stages are driven from a ±10 V output from the Geo Brick using a 16- or 18-bit output where appropriate, and the interferometer is read using an incremental or absolute BiSS-C interface. Scans that are within the range of the piezo

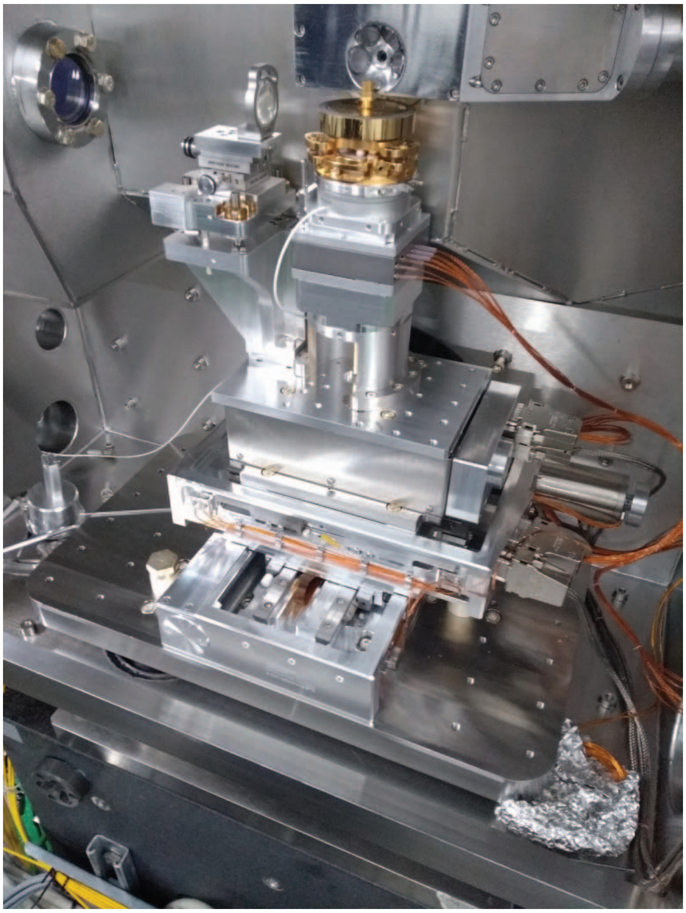
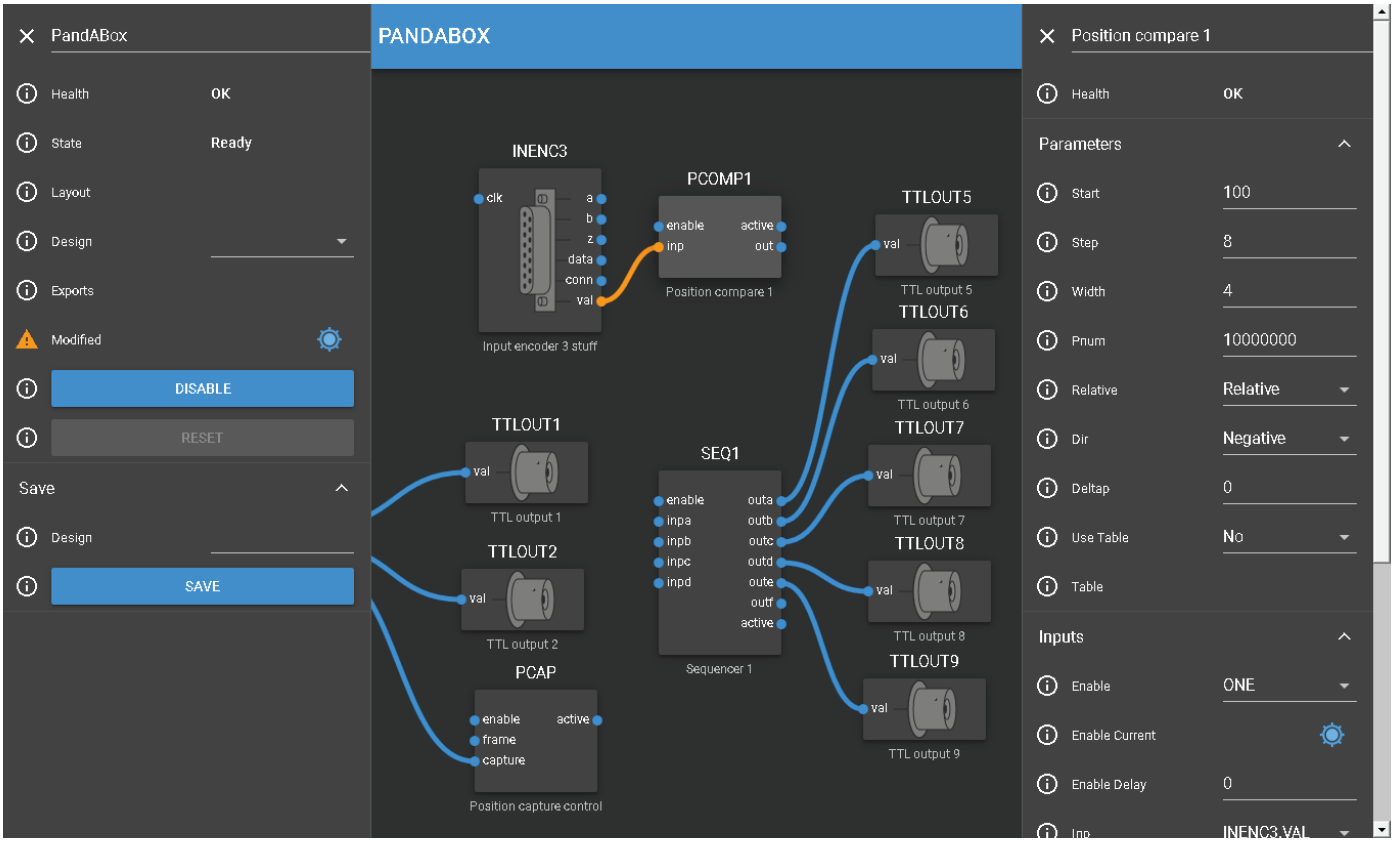


Figure 2: The stage stack from the I14 beamline. The XY coarse stages can be seen at the base of the stack, with the fine piezo stages being the grey block towards the top. The lenses to the left of the sample position at the top of the stage are for the interferometer encoders. Much of the other equipment is for cooling and sample handling.



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Enable	ONE
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Enable Delay	0
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Figure 3: The PandABox configuration interface showing how FPGA functional blocks can be "wired up" at runtime.

move just the piezo, with larger scans moving the coarse stage while using the piezo to smooth the combined motion.

PandABox

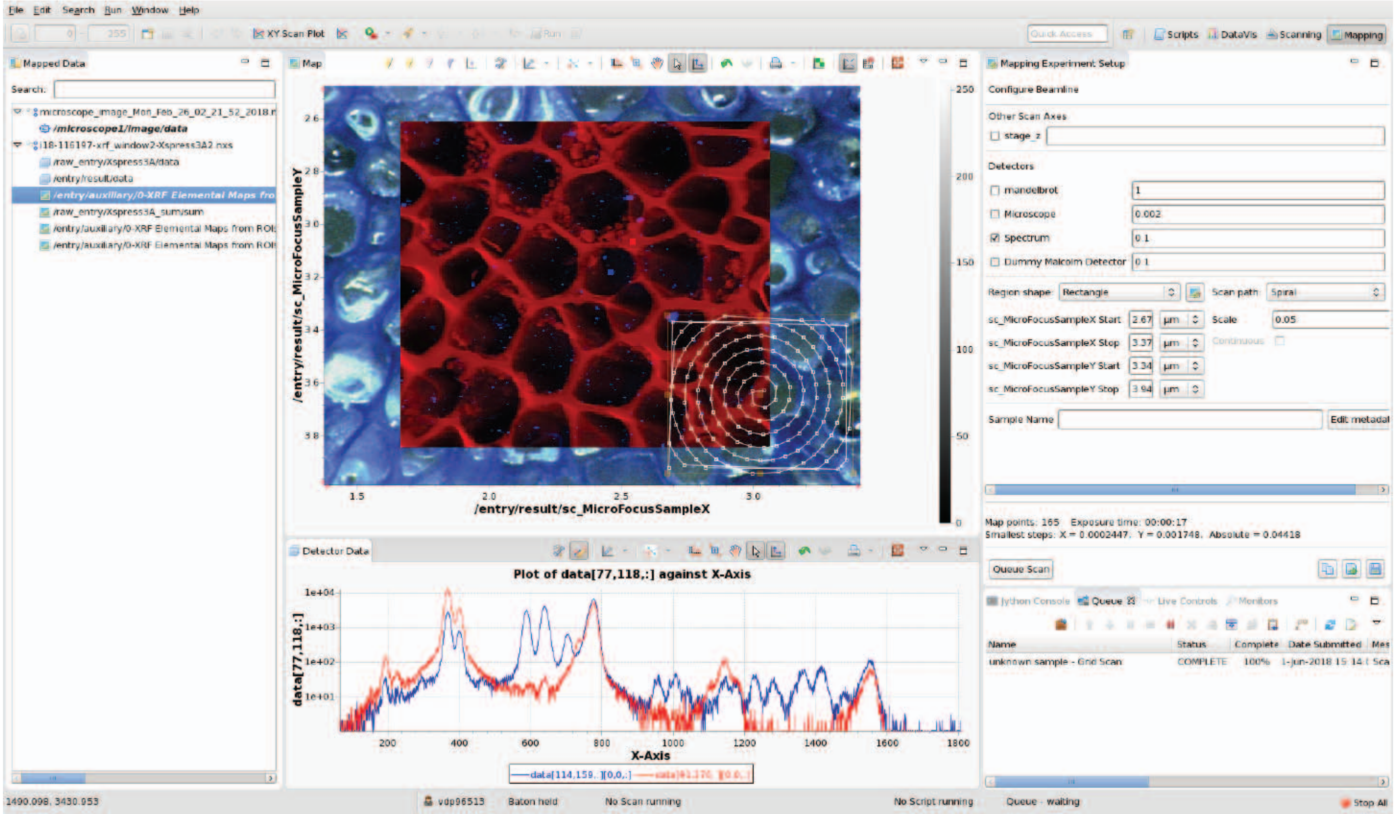
To properly orchestrate a hardware scan, and mitigate the memory limitations involved in rapidly and synchronously capturing encoder positions to the Geo Brick, the PandABox was developed [7]. This is a highly flexible FPGA-based hardware project in collaboration with SOLEIL, commercialized by Quantum Detectors. It is currently used to capture encoder positions when triggered by the Geo Brick, but can also be used to generate arbitrary streams of pulses in response to a mix of external triggers, position compare on encoders, and time delays.

Malcolm

Malcolm [8] is a new piece of software developed in Python specifically for this project. Malcolm is effectively a middle layer between the data acquisition level and the EPICS and hardware layer that focuses on conducting hardware scans in a generic and extensible way. Malcolm is comprised of several parts, and is designed to map in software the hardware reality on the beamline. If there is a Geo Brick controlling the stages, with the stages encoders fed through a PandABox, and the appropriate triggering also connected, as well as a hardware triggerable detector which is also connected to the PandABox, then the Malcolm configuration should reflect that. Malcolm was designed at the start of the project to deal with making a scan performant, and to do it well, but to be aware of other elements that could be happening in a scan, such as additional scan axes such as energy or temperature, which are outside the control of Malcolm.

GDA

The Generic Data Acquisition (GDA) [9, 10] system at Diamond is the main user interface for the beamlines. This project added a lot of new functionality to the GDA in the form of a new scanning mechanism which is compatible with Malcolm, and writing NeXus files with the high level of metadata described earlier. Much work was also done on UI elements to allow the setup and control of a hardware mapping scan. GDA's role is to orchestrate experiments at the scientific level, and to send back scientifically relevant information to the users of the system. In this work, GDA has a critical role at the heart of the project. This is where the user selects the region of the sample that he or she wants to scan, and decides parameters for the scan and the path of the sample. It also allows them to specify other parameters to scan as part of the experiment, commonly things like beam energy or sample rotation. When the scan is running, the GDA makes use of SWMR to visualize the data as it is collected, and interactively display this to the user. The GDA



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Configure Beamline

Other Scan Axes

☐ stage_z

Detectors

☐ mandelbrot 1
☐ Microscope 0.002
☑ Spectrum 0.1
☐ Dummy Malcolm Detector 0.1

Region shape: Rectangle
Scan path: Spiral
sc_MicroFocusSampleX Start 2.67 µm
Scale 0.05
sc_MicroFocusSampleX Stop 3.37 µm
Continuous ☐
sc_MicroFocusSampleY Start 3.34 µm
sc_MicroFocusSampleY Stop 3.94 µm
Sample Name

Map points: 165 Exposure time: 00:00:17
Smallest steps: X = 0.0002447, Y = 0.001748, Absolute = 0.04418

Name	Status	Complete	Date Submitted	Mes
unknown sample - Grid Scan	COMPLETE	100%	1-Jun-2018 15:14:(	Sca

1490.098, 3430.953 vdp96513 Baton held No Scan running No Script running Queue - waiting

Figure 4: A screenshot of the GDA showing many of the different software elements combined. The panels to the right are GDA-specific and deal with setting up scans and associated processing. The panels to the center and left are DAWN visualization components which allow microscope images and multiple hyperspectral data blocks to be visualized. In the center panel, a spiral scan trajectory is plotted making use of the Scan Point Generator system.

can also be used to set up processing to occur on the frames as they are collected, or define processing on the fly to be applied to the data. The results of this live processing are also fed back to the user interface, allowing for interactive live processing. The GDA also has the ability to link directly to EPICS area detectors and display the live MJPEG stream, or the slower but higher-detail full array.

Scan Point Generator

Another custom piece of code which was developed specifically for this project was the Scan Point Generator [11]. This is a piece of pure Python code which fully describes scan patterns that may need to be created. For example, if the users want a spiral pattern scan, where each point is offset by a random amount, and it is constrained to be within an arbitrary polygon, they can specify this. It is important that it is pure Python, as it is used by Malcolm to conduct the created scan paths, but such complicated paths need to be set up in the GDA UI. The GDA is a Java application, but has access to Jython where needed. To make sure that the same points are shown on the UI as are actually specified to the scan, we made sure that the same code was responsible for each. This led us to take such steps as writing specific random number generators, as the underlying libraries provided different results otherwise.

DAWN

DAWN [12, 13] is a sister project to GDA, in that they are both written using the Eclipse RCP environment and share many components. All of the visualization elements that are available in GDA for viewing the live data are also available in DAWN for visualizing after the data have been collected. The visualization of complex data is made possible by careful interpretation of the NeXus metadata, and this data management is dealt with by the January suite of dataset classes and tools [14]. During the project, considerable work was undertaken to extend all of these existing systems to fully support SWMR, as well as to best present the multiple datasets collected in many mapping experiments.

DAWN also deals with all of the processing that needs to be undertaken during the scan [15]. The DAWN processing framework undertook significant upgrades to make it compatible with SWMR; this means that any processing that is available through DAWN is also available live during the data collection in GDA [16].

Beamline summary and results

In this section, we detail the beamlines on which the proposed system was installed and tested.

P45 test rig

As part of this project, it was considered important to have a mock system which could be used for testing prior to going live on a beamline. The P45 test rig was created to do exactly this; the system has a standard Geo Brick, PandABox, and area detector setup, and simple stages so that real hardware scans can be achieved and tested. In addition, the full standard beamline compute infrastructure is available to test software deploys. Although simple, this test system allowed us to fully explore many of the components of the project in a safe environment before going live, and although this did not fix all bugs, many were identified before getting to the beamlines.

I18

I18 is one of Diamond's Phase I beamlines, and specializes in microfocus mapping and spectroscopic experiments. The beamline is used in all areas of science; the major areas are investigating trace elements in biological tissue (e.g., metal dysregulation in neurodegenerative diseases [17]) and understanding the cycling of elements in geoscience (e.g., selenium in shales [18]). Attempts had previously been made to X-ray fluorescence (XRF) map quickly (>10 Hz), but this was challenging as the detector was read out between rows. This file reading/writing dead time (ca. 10s) needed to be eliminated in continuous XRF scans for greater efficiency and to enable greater use of XRF tomography and XANES mapping; hence, it was included in the Mapping Project. The biggest challenge with I18 was that, as an established beamline, there were clear expectations of the essential deliverables, as the beamline performance needed to improve after the upgrade.

Now, the beamline is achieving significantly faster scan speeds (200 Hz), with dead time <1 s between rows [19]. There is also a clear pathway to increase these speeds to kHz and beyond with continued development in the core technologies.

I08

The I08 beamline at Diamond is a soft X-ray SXM beamline. This beamline originally used a commercially available Bruker endstation, but with the flux available on the beamline, plans were made to increase the performance using a custom sample stage setup. This new stage setup required new software and hardware, and so it made sense to include it in the project. I08 makes use of a photo-diode as its primary detector, so it can run very quickly. Currently, the motion is limited to 300 Hz; however, similar to I18, there is a clear path to achieve kHz scanning.

I14

The I14 nanoprobe beamline has just gone into operation and is essentially a nanoprobe version of I18, but with the nanopositioning complexities of I08. The main purpose of this project was to provide I14 with a system to control the beamline scanning mechanism, which is feature-rich and performant. As I14 had no other solution, there is no direct comparison to an existing system; however, the new system has been operating at up to 100 Hz for XRF and XANES mapping on the beamline.

I13-1

I13-1 is the coherent imaging beamline at Diamond [20] and, as a well-established beamline, already has a very effective scanning mechanism. It was included in the project because it had some unique requirements for a scanning system, as it routinely performs ptychography experiments. Ptychography is a Fourier-transform-based technique. An interesting artifact that occurs in the resulting reconstructions comes from introducing regular features in the sampling, such as collecting the map on a regular grid. This is commonly handled by sampling with a non-regular pattern, such as a randomly offset raster or a spiral pattern; the requirement is to hardware scan in a non-regular way, but in a generic enough way to be adopted elsewhere.

Currently, I13-1 has tested the new mechanisms, but is still using alternative scanning to maintain a high-quality service. There are plans in place to migrate to the new system over the next few years when the ODIN upgrades to Excalibur are available.

I05-1

I05-1 is the nano-ARPES beamline, and like I13-1 was chosen as it brought different elements to the project, such as different detectors and requirements. This was important, as it meant that the project was not focused only on mapping XRF experiments, and was kept more general. I05-1 was, like I14, a new beamline with no existing solution, so this made it a good candidate, especially as it has the same nanopositioning problems as I08 and I14. The mapping at I05-1 inherently involves detection in 2D (angle, energy) space, so here the mapping project was a priority to achieve fast and reliable 4D imaging in direct and inverse space. The test experiments demonstrated improvement in acquisition speed by a factor of 10 with implementation of low-level synchronization in Malcolm.

Future work and extensions

We look to exploit the original requirement to be able to conduct any trajectory scan to perform fast, high-quality ptychographic measurements. Since ptychography also works using visible light [21], we have extended the concept of the P45 test rig to allow an end-to-end working experimental system. This will enable data collection strategies to be investigated and processing to be checked with real data rather than just simulations or pre-scanned data.

The P99 optical development rig is a self-contained system which is computationally identical to a standard beamline, including the core equipment and software discussed earlier. With a laser-based optical setup (Figure 5), and the electronics and computing housed in a single rack, we now can truly repeat the same software bugs as a beamline without requiring SR. We can also record real data, which can be processed identically to SR data. This is incredibly important for our ptychography application, as the data collection and reconstruction are closely coupled. Further details of the full scope and features of this rig will be given in an upcoming article, and its use in the extensive development of Diamond's Dual Imaging and Diffraction (DIAD) and J08 (soft X-ray ptychography) beamlines.

Conclusions

This article briefly covers the combination of software and hardware decisions which make up Diamond's Mapping Project with nanoposition-

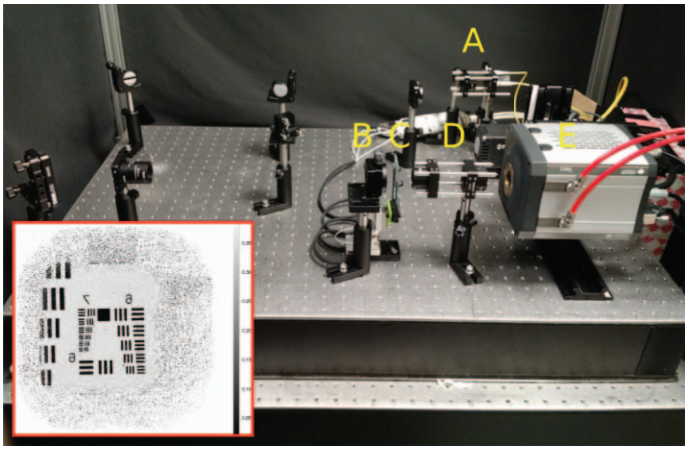

Figure 5: The P99 test beamline showing: (A) the fiber-coupled diode laser illumination (currently commissioned for λ = 630 nm and λ = 405 nm); (B) 25 mm condenser lens; (C) sample mounted on 3 axis Smaract SLC stage, controlled by SDC2; (D) variable configuration post-sample telescope; (E) Andor Neo 5.5 controlled by EPICS Andor 3 driver. Inset: magnitudes of the first prototype ptychography reconstruction from this rig using Ptypy [22] for analysis and the mapping software to collect the data via a 30 Hz spiral hardware step scan.

ing capability, and how these technologies have been applied to several of the X-ray micro- or nanoprobe beamlines at Diamond. The work has generally been seen as a success, with several follow-up projects in consideration for extending the technology stack to other areas, such as ptychography, tomography, and macromolecular crystallography. The system is capable of conducting fly scans at 300 Hz with every position uniquely defined. Step and dwell scans are also possible at this speed if the hardware allows, although usually jitter in the motors is prohibitive at these speeds. As the Delta Tau Geo Brick is used for motion control, many motor systems can be connected using a selection of available modules.

Several elements of the system were specifically created for this project, as no existing, compatible solution was available. Creating software from scratch is not taken lightly, and hardware doubly so, but all of the items developed here have been produced with an eye on long-term sustainability. Most of the software elements of this project are available under permissive open source licenses, and those that are not are looking to transition in the near future.

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Note