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P99: AN OPTICAL BEAMLINE FOR OFFLINE TECHNIQUE DEVELOPMENT AND SYSTEMS INTEGRATION FOR PROTOTYPE BEAMLINE INSTRUMENTATION

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Abstract

We present a beamline analogue, capable of system prototyping, integrated development and testing, specifically designed to provide a facility for full scientific testing of instrument prototypes. With an identical backend to real beamline instruments the P99 development rig has allowed increased confidence and troubleshooting ahead of final scientific commissioning. We present detail of the software and hardware components of this environment and how these have been used to develop functionality for the new operational instruments. We present several high impact examples of such integrated prototyping development including the instrumentation for DIAD (integrated Dual Imaging And Diffraction) and the J08 (Soft X-ray ptychography) beamline end station.

INTRODUCTION

Diamond Light Source is a publicly funded 3rd generation national synchrotron soon to boast 39 operational state-of-the-art user accessible instruments covering a wide range of physical and life science applications. Such instruments pose a large number of challenges from initial scientific concept, to final user experience. To get best efficiency and value for money, Diamond operates a modular approach for engineering and software systems support, usually with each custom hardware or software component coming together on the final instrument in-situ. This can be a high-risk strategy with any issues arising during the final scientific commissioning of the beamline. This is often unavoidable due to the bespoke nature of the instruments. Small prototyping rigs for instruments have been used to some success, but often do not consider the underlying infrastructure, or are focussed on only specific sections of the software/hardware stack, which have been identified as problematic. Such approaches risk ignoring the complete user/operator experiences.

P99 is a collaborative offline testing facility that aims to tackle such shortfalls by providing a space for collaboration and innovation amongst support teams and beamline staff. Such prototyping allows a degree of confidence to be established in the building blocks of otherwise complex and multifaceted projects. A laser-based analogue to a real beamline, P99 is specifically targeted at cases that either 1) target the full software stack requiring a full beamline infrastructure backend for testing, 2) require a high brightness/coherence source with high speed triggering 3) require high stability i.e. for nano-positioning use cases.

In this manuscript we introduce the design of P99 and show 3 case studies where this facility has allowed testing of multiple prototypes across multiple instruments (DIAD [1], J08 [2]), and current ongoing ptychography [3, 4] developments facilitating collaboration and prototyping across groups of the instrument as a whole well in advance of the final deployment, allowing issues to be realised and approaches refined.

P99 DEVELOPMENT RIG

The P99 development rig is identical in networking, compute and controls infrastructure to a true user facing instrument. This means that any solution developed on P99 should work equally as well on a user beamline/instrument making P99 unique compared to other such testing facilities at Diamond. This infrastructure is housed in the rack in Fig. 1 and is compliant with the architecture described in [5] and so can make full use of this work.

Figure 1: P99 optical development rig in the precision metrology laboratory, complete with main and small testing rack, opaque enclosure and beamline workstation.

P99 is situated in Diamonds precision metrology laboratory [6], with a foundation of an actively damped honeycomb optical breadboard. Inside of an acoustically damped, opaque enclosure (Fig. 1), there is a secondary breadboard, which is isolated from the actively damped breadboard by Sorbothane pads. This is similar in design to many Diamond instruments, and ensures that the secondary breadboard is stable to the nanometer scale. Aside from stability, another benefit of being located in the precision metrology laboratory is the proximity to other like-minded projects that exist across Diamond.

The light source used is a fibre-coupled diode laser (Thorlabs MCLS), of which predominantly the blue (405nm) and red (632nm) outputs are used. A variety of 1" optics, combined with vibration isolating posts are used to create optical set-ups that are analogues of the more complicated X-ray set-ups of the user-facing instruments. Tests predominantly use the Andor Technology detectors that cover both the SDK2 and SDK3 functionality, which are widely used at Diamond.

CASE STUDY 1: DIAD BEAM SELECTOR

Diamonds novel DIAD (Dual Imaging And Diffraction) beamline utilises two X-ray beams (Fig. 2a), split after the source, to allow simultaneous morphological imaging via radiography/ tomography, as well as mineralogical/strain information gathered via the process of X-ray diffraction imaging. This beamline will have high impact across a broad spanning range of both in and ex-situ samples across the physical sciences.

Such a state-of-the-art beamline presents many instrumentation challenges. One use case on DIAD includes fast switching between radiography and diffraction at 10 Hz. Beam selection is required to stop cross contamination of the beam from one technique to the other, e.g. the imaging beam causing interference with the diffraction data on the diffraction detector.

To facilitate this fast beam selection, the beamline staff and engineering team designed a switching mechanism utilising a bespoke rota (Fig. 2 inset), designed so that that rota can be manipulated in vacuum by an ex-vacuo motor through a rotary seal. In order to achieve their primary specification of 10 Hz selection rate, a high power motor (Kollmorgen, KBM-17H01-C-00) was selected. In order to synchronize the movement of the beam selector with the two detectors for arbitrary trigger patterns it was suggested to implement hardware triggering using pyMalcolm [7], combined with a Quantum Detectors PandABox technology; a system that has worked well in a parallel use case of high speed mapping. With the beamline not due to take beam for 2-3 years after this initial design, and further confidence in the design desired, it was decided to test this equipment on P99.

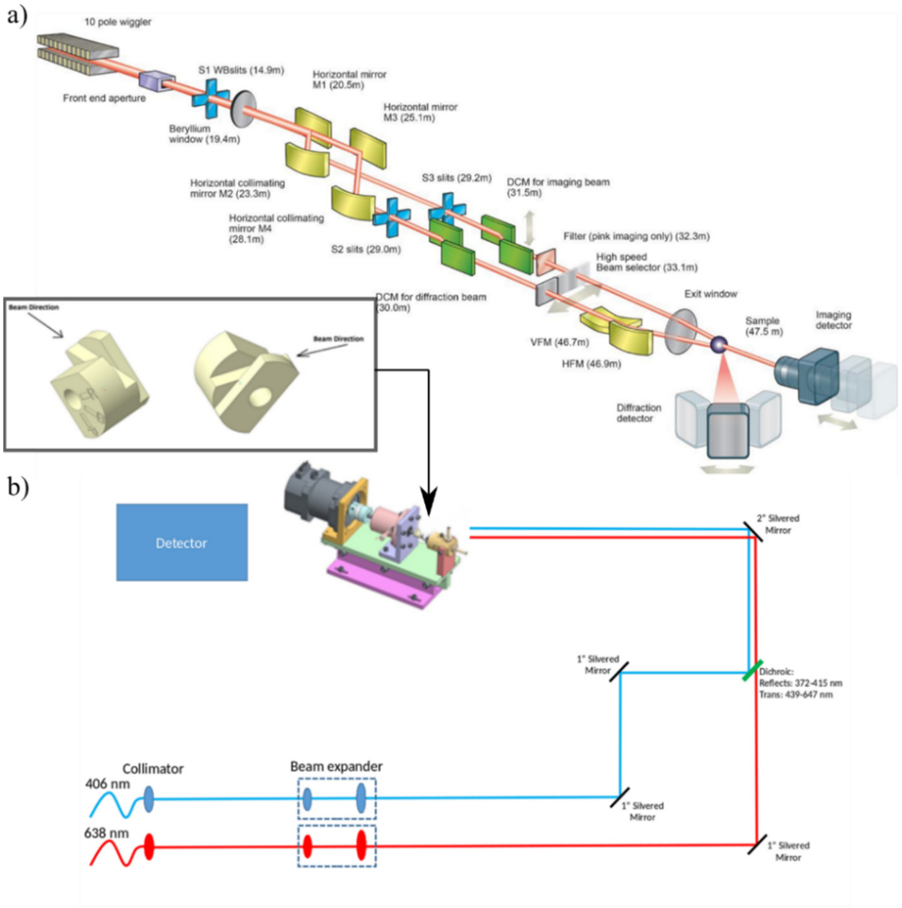


Figure 2: a) Beamline layout for DIAD (Dual Imaging and Diffraction beamline) showing configuration for two beams split after the source. b) Configuration for testing the beam selector showing two independent laser beams

To mimic the specification of the DIAD beamline in the lab it was decided to use two collimated laser beams, one blue (405 nm) and one red (638 nm) brought on to a parallel beam path as shown in Fig. 2b. The beam selector was aligned as per the mechanical design (shown in Fig. 3a), and control software implemented. An Andor Technology Neo 5.5 sCMOS detector was used in external trigger mode to detect the optical light in place of the beamline detectors which respond to X-ray energies only. The output triggers from the PandABox were linked to this detector by a logical OR to keep as much of the system the same as the final design as possible.

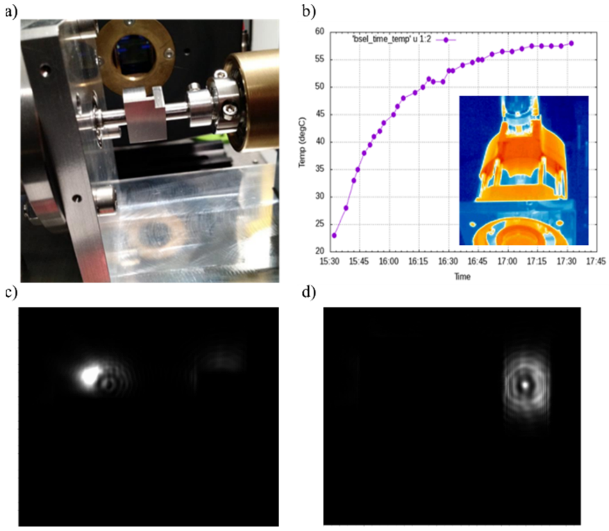


Figure 3: a) The DIAD beam selector aligned to the beam. b) Thermal image of the main drive motor running at 10 Hz as it will be finally used showing equilibrium at 60 C. c) Image on detector with Imaging beam selected d) image on detector with diffraction beam selected

After initial testing it was found that the system was unable to meet the 10Hz switching desired (Fig. 3b). The reason for this was found, after motor tuning, to be that the power supply for the motor was unable to generate a high enough current to stop the motor abruptly enough. Replacing the power supply with a Blade PSU and tuning the motor current limits allowed each beam to be imaged at the required 10 Hz. Some drift in encoder position was also noted and discounted since the required beams were not occluded (Fig. 3c) and 3d)), and the software stack testing was completed by demonstrating the implementation of the beam selector in the GDA acquisition software [8].

Finally, by installing a thermal imaging detector targeted at the motor, it was possible to check that the motor would not overheat with this higher current power source running in operation conditions and instead stabilised asymptotically at 60 degrees suggesting a further cooling strategy was not needed.

Such early testing of this prototype allowed confidence to be developed in the design of this novel piece of instrumentation well ahead of the beamline build.

PTYCHOGRAPHY

Ptychography is a computationally intensive scanning microscopy technique that allows resolution of detail beyond that of the regular point spread of a STXM. Combining information about the scanning trajectory with area detector images relating to the Nyquist sampled area inside the beam ptychography is able to cope with a multitude of aberrations and imperfections in the raw data. Ptychography allows a compromise between hardware and software, where the computational complexity in analysis can be increased to trade-off with hardware/control system limitations.

Delivering ptychography to more than one beamline at a facility requires both beamline specific (with regards to end station design and scientific focus) and also beamline agnostic approaches (frameworks which make the most of the infrastructure).

The following two case studies demonstrate Diamonds strategic use of P99 for both of these approaches in both the build, testing and development of the end station for Diamond novel soft X-ray Ptychography beamline (J08), and the testing of both controls, and analysis infrastructure to cope with both acquisition of high quality data at high rate, and processing of the huge data volumes in a way that is both extensible and maintainable.

Case Study 2: J08 – Soft X-ray Ptychography Beamline End-Station

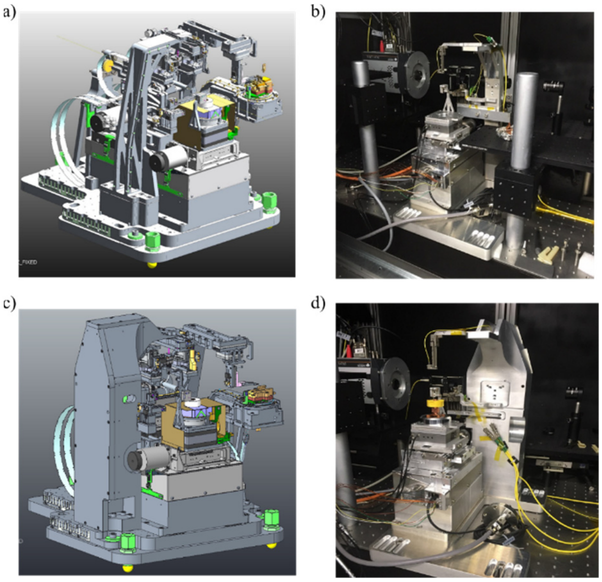


Figure 4: The stage and interferometer system design (a and c) and implementation on P99 (b and d) for both old and new reference arm designs respectively.

J08 is a new state-of-the-art scanning microscopy beamline, which aims to be available to users in 2020. Building on the work of the adjacent I08 scanning X-ray microscopy [9], J08 plans to use ptychography to image a wide range of physical and biological samples to sub 10nm resolution using soft and tender (200eV – 2000eV) X-rays. The beamline plans to roll-out support for both cryogenic and tomographic imaging as it ramps up user operation.

Such a high resolution scanning microscopy system requires a high degree of control over, and information about, the positions of the stages. The systems mechanical design consists of a coarse XY stepper motor stack (PI-Micos) underneath a fine control flexure stage (Piezo Jena Tritor 101). Feedback for the position of this combined motor-system is provided via an Attocube IDS interferometer system with sensor heads mounted on an independent reference arm.

Building on existing, static tests of the mechanical setup the decision was made to install a duplicate of the sample motion stack on P99 to study how it behaved dynamically as shown in Fig. 4, allowing such tests to take place up to a year before the X-ray commissioning of the final end station. The control system was set-up with the software stack demonstrated in [5] with the detector chosen being an Andor Technology detector which uses the SDK2, the same as that which will be used as an initial detector on J08. The system was investigated under continuous scanning, with a target of 5 nm noise on the following error. Although it is possible to correct for positional errors/ incoherent states in ptychography [10-12], in house analysis investigations have shown that the computational cost for fixed ptychographic reconstructions time increases linearly with the incoherent blurring kernel introduced by, per pixel, noise in the position of the stages relative to the beam. Since modern scientific user measurements require feedback that is close to real-time in order to allow experiments to be guided, it is essential for high positioner performance under measurement conditions.

Although this investigation is still in progress, initial results from the testing have proved positive. Initially noise in the position of the sample using the flexure stage was between 15-30 nm (Fig. 5a). This was initially suspected to be due to errors coming from the lack of stiffness in the design of the interferometer reference arm, against which the positions are recorded. To test this hypothesis, a stiffer reference arm was designed and constructed. Initial tests against the background have shown an improvement in the fixed position error of a factor of 3-4 (Fig. 5b-c). This has translated into a smaller build-up of following error in continuous moves.

The impact of this improvement in the downstream analysis will translate directly to a factor of 3-4 reduction in the required compute to process the result in a fixed feedback time.

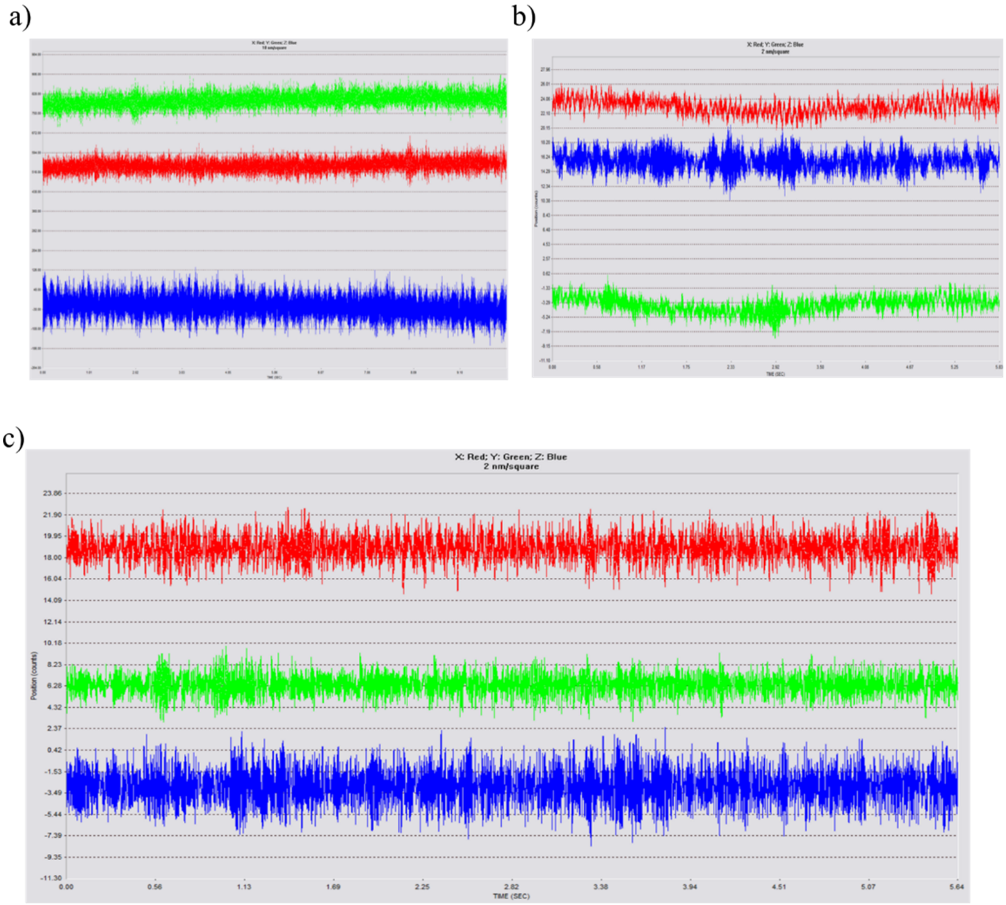


Figure 5: a) Background noise of old interferometer reference arm, grid: 10 nm. X (red) ±6 nm, Y (green) ±6 nm, Z (blue) ±15 nm. b) Background noise with new reference arm, grid: 2 nm. X (red) ±2 nm, Y (green) ±1.5 nm, Z (blue) ±4 nm. c) PID loop turned on, grid: 2nm. X (red) ±2 nm, Y (green) ±1.5 nm, Z (blue) ±4 nm.

The next stage of this investigation is to demonstrate similar behaviour when the stage is manipulated via the control and acquisition system and to progress the final implementation in the J08 end station.

When this is underway the hope is to be able to use the same prototype to develop the controls system for use in scanning ptychography-tomography; an additional, very challenging apparatus implementation.

Case Study 3: Diamond Ptychography Project

The Diamond ptychography project aims to bring close-to-real-time ptychography measurements to 5 state-of-the-art instruments (I08, J08, I14, I13, ePSiC) in the Imaging and Microscopy Science Group [13]. This project differs from the other two case studies since it is an infrastructure project, concerned with upgrading the core capabilities of the controls and analysis software so that they may better cope with the move towards making ptychography on these instruments a measurement rather than an experiment.

To achieve this, the controls software must be developed to be able to achieve movements and framerates synchronized to 10 kHz. This will provide a large amount of data, which needs to be analysed and displayed back to the user interface as quickly as possible so that science users may guide their investigations.

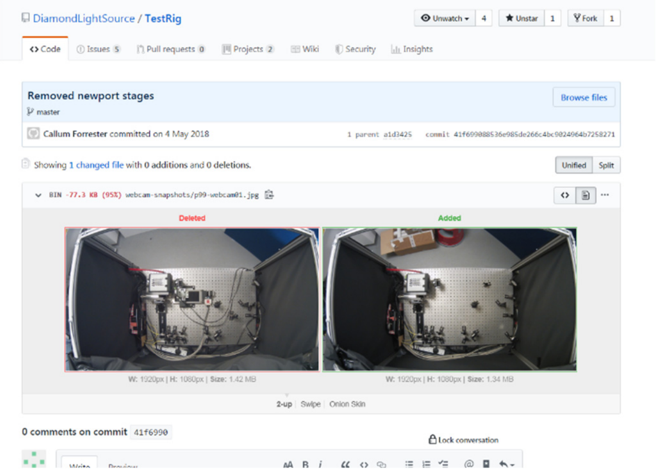
To keep the developments close to the beamline and create confidence in the results, it was decided to test the progress on P99. Since these developments are closer to the core software than the hardware it was decided a simple Smaract SLC 3 axis motor would be best to be used to manipulate a simple USAF test sample. In keeping with previous developments, it was decided to use Andor Technology detectors covering both SDK versions.

This project is still in progress, but has been used to test control system developments including: upgrading pyMalcolm version, moving Diamonds infrastructure from Redhat (el6 to el7), bug fixing and test of both Andor Technology SDK's, introducing features so that hardware triggered scans may be paused and re-wound (allowing pausing for machine top-up), moving towards a position compare trigger system that will allow acquisitions up to 10 kHz. From the analysis side, a Zocalo [14] pipeline has been developed to kick-off the reconstruction at the end of the scan from an NXcxi_ptycho [15] application definition. We are using a combination of DAWN (Data Analysis Workbench) [16] and the Ptypy [17] frameworks to handle the data processing, and updating the latter to be GPGPU (General Purpose Graphics Processing Unit) enabled.

CONCLUSIONS AND OUTLOOK

We have introduced the P99 optical development rig for use in testing and prototyping equipment for real beamline end-stations and equipment. P99 has improved confidence in the design and operation in the 3 case studies shown, and continues to be oversubscribed in future work. The hope is that the rig will grow, supporting additional software and hardware branches.

After the existing branches have been used to develop against, they will be adapted to be used for hardware (Fig. 6) and software version control. The concept of Hardware version control is one that is used regularly now on P99 and utilises a webcam to track hardware changes through different set-ups. GitHub provides a useful interface to take the difference of these images, allowing previous breadboard designs to be compared in-line with the software. We plan to extend this functionality through nightly builds of the latest software developments being run and stress tested on this real-life set-up with a hope to improving the long term stability of the full software stack across all Diamond beamlines.



DiamondLightSource / TestRig

Removed newport stages

master

Callum Forrester committed on 4 May 2018

1 parent a1d3425 commit 41f699088536e985de266c4bc9024964b7258271

Showing 1 changed file with 0 additions and 0 deletions.

BIN -77.3 KB (95%) webcam-snapshots/p99-webcam01.jpg

W: 1920px | H: 1080px | Size: 1.42 MB

W: 1920px | H: 1080px | Size: 1.34 MB

0 comments on commit 41f6990

Figure 6: Hardware version control shown via GitHub diff of image from overhead webcam (https://github.com/DiamondLightSource/TestRig/blob/master/webcam-snapshots/p99-webcam01.jpg , commit hash:41f6990)

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