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Automatisation developments on ESRF-EBS BM05 beamline

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Abstract

X-ray computed tomography and radiography imaging are currently the second most exploited technique at the European Synchrotron Radiation Facility (ESRF) for commercial services. To maximise the growth, the beamlines must be flexible enough to accommodate a wide range of materials and sample sizes, whilst conserving operational efficiency and ensuring reliable and high-quality imaging outcomes. In this paper, we present some of the latest developments on the BM05 tomography beamline from the ESRF in terms of automatisation, processes, and procedures that ensure an efficient and robust operation of the beamline. For all users, the automatisation developments are focused on being able to set-up the beamline in a pre-defined state as easily and quickly as possible, so that time consuming user interventions (and potential mistakes) are minimised. For academic users, a graphical user interface (GUI) called *Daiquiri tomo* has been developed as a simple tool for non-experts to be able to perform most of their scanning operations in a user-friendly and efficient fashion, with minimum support from beamline scientists. For commercial users, a robotic sample changer has been assembled to be able to scan series of up to 45 samples, and maximise usage of night shifts. Overall, those improvements are key in reaching operational excellence and X-ray computed tomography and radiography imaging are projected to rival macromolecular crystallography (MX) as the first technique for commercial services at ESRF by the end of 2025.

Keywords: SRCT, synchrotron radiation, GUI, automatisation, quality assurance

More info about this article: https://www.ndt.net/?id=30764

1 Introduction

As of March 2022, a critical mass of beamlines having tomographic and radiographic X-ray imaging as their core business are now operational at the ESRF: BM05 (small field of view, high resolution, medium energy, microtomography), BM18 (large field of view, high energy, HIP-CT), ID19 (high speed microtomography and radiography), ID16 (nano-imaging), ID15 (high energy, ultra-fast tomography), ID06 (diffraction contrast tomography, dark field), ID11 and ID31 (diffraction contrast tomography) [1]. This portfolio of beamlines would benefit from a strengthened interoperability, enabling more efficient support and local contacting for both industry and academics users. Moreover, it is an opportunity to bring the ESRF's tomography industrial user services and support up to the standard expected and demanded by commercial clients already today**,** and in preparing the future. This latter is particularly important as tomography is being used for commercial work at increasingly higher technology readiness levels. At this level of service, standards and quality control play a role in ESRF services being compatible with**,** and exploitable by industrial needs. The interest from industry for quality approaches has been highlighted in a recent workshop [2] on the potential added value for quality assurance in commercial synchrotron services.

Since ESRF EBS (Extremely Brilliant Source) upgrade in 2019, beamline BM05 is a 2-pole wiggler beamline equipped with experimental stations to perform X-ray tomography, topography, diffraction, reflectometry and wave front metrology. Beams of decimetre to micrometre sizes and energies from 6 keV to 150 keV are available for industrial use and for developing the instrumentation of the future [3]. X-ray tomography is available on BM05 for both academic (through proposals twice a year) and industrial (faster and paid access) experiments. BM05 has a high automation level suited for high throughput and is equipped with a sample changer. With up to 3.5 metres for propagation phase-contrast, BM05 proposes a large range of polychromatic beam energies (25-150 keV) and pixel sizes (0.36-25 µm). To cover such a wide range of pixel sizes, 3 optic systems are available (see Figure 1):

1. **Dzoom:** continuous covering of the range 6.5 µm pixel size up to 25.5 µm. Only one scintillator type, LuAg(Ce) 1000 µm thick with or without reflective coating. Pco.edge 4.2 CLHS (Camera Link High Speed) sCMOS camera (2048 x 2048 pixels) [4],
2. **Zoom:** continuous covering of the range 3.0 µm pixel size up to 5.7 µm, Three scintillator available, all LuAg(Ce) with reflective layer, with thicknesses of 100 µm, 500 µm, and 250 µm. Pco.edge 4.2 CLHS (Camera Link High Speed) sCMOS camera (2048 x 2048 pixels),
3. **Twinmic:** three objectives available for 3 fixed pixel sizes: 5x objective gives 1.44 µm pixel size, 10x is 0.72 µm, and 20x is 0.36 µm. Only two objectives can be mounted at a time, usually the 10x objective is the fixed one, the other one swaping between 5x and 20x objectives. Three scintillator types are available, LuAg(Ce) 50 µm thick, LSO(Ce) 23 µm thick, and LSO(Ce) 8.8 µm thick, all without reflective coating. Pco.edge 4.2 CLHS (Camera Link High Speed) sCMOS camera (2048 x 2048 pixels).

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Here, we provide a snapshot of the beamline in February 2025, and present the steps taken towards enhancing operational efficiency by improving beamline flexibility whilst ensuring reliable and high-quality imaging outcomes.

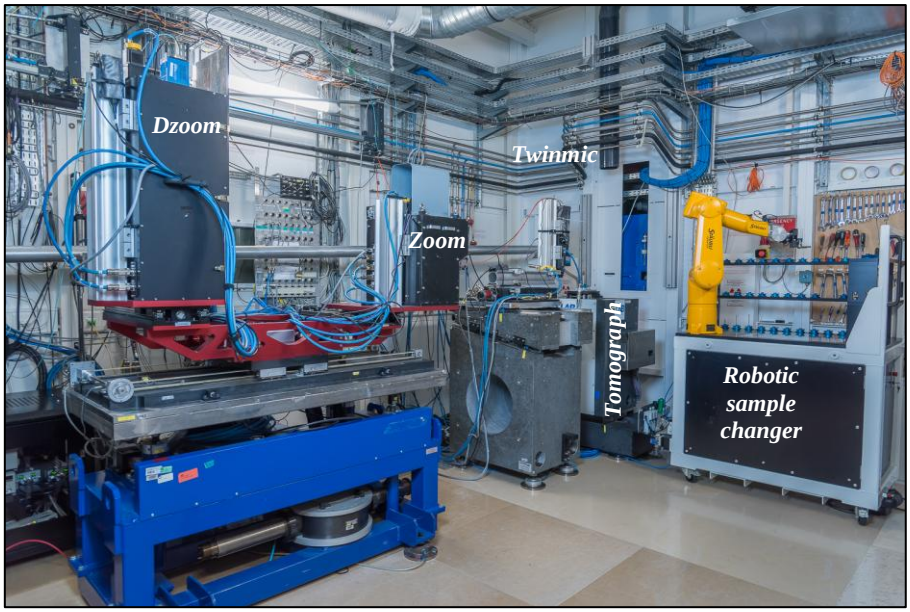

Figure 1: Photography of BM05 experimental hutch 2, with the tomohgraph, the 3 detector optics (Twinmic, Zoom, and Dzoom) and the sample changer. (Courtesy of IRT Nanoelec)

2 Developments

Beamline BM05 at the ESRF is an X-ray computed tomography beamline that covers the energy range 25-150 keV and voxel size range 0.36-25.5 µm. For each measurement, the camera (selected from one of the 3 different optic systems available) must be centered on the beam, slits must be moved to crop the beam and define the region of interest (ROI); the beam energy, propagation distance and pixel size must be adjusted; and the sample centered within the ROI. As all these operations can be complex and time consuming, and must often be repeated, for example when changing pixel size, this section presents the recent developments made on BM05 to automatise some of these operations and thus maximise efficient and robust operation.

2.1 Procedures & automatisations

Performing a tomography experiment on a synchrotron beamline requires the following steps:

1. alignment of the optics system and stage
2. centering of the sample and selection of the field of view FOV (or region of interest ROI when doing local tomography)
3. optimisation of acquisition parameters

which can be an iterative process.

For the first step, the macro *alignment* takes an image of a reference absorbing sample with 2 edges at 0° and 180° in order to set the position of the sample stage rotation axis (*y* translation under the rotation stage) centered onto the detector and also correct for any rotation of the camera to set the rotation axis exactly parallel to the middle column of the camera. The macro can be run multiple times, until the correction values for rotc are below 0.01° (1 pixel over 2048) and below 1 pixel for *y* translation. Next, the macro *focus_retune* can be used to adjust the focus of the camera (meaning adjusting the scintillator position to the objective working distance). This macro is a high-level script that calls the refocusing macro specific to the currently active detector, using objects adequate to each detector. The pixel size can then be determined with the macro *measure_pix*, which takes images of the same reference sample displaced by a known amount (60 % of the field of view for example). The macro provides a value of the measured pixel size along with a graph of the correlation between the two images.

For alignment and centering of samples, the macros *align_jar* and *easycent* can be employed. *Align_jar* is used by defining the left edge of the sample for 0°, 90°,180°, and 270° of rotation to automatically centre the sample within the current field of view (FOV), especially useful for samples bigger than the FOV (local tomography). *Easycent* is used on a reconstructed slice. The user simply clicks on the point/feature of interest, which is put in the centre of the camera FOV (sample is moved along *x*, *y*, and *z* axes). It is also possible to select a given point and move it to a specific position within the FOV, this is useful when wanting to scan complicated sample areas such as corners of a cubic sample. Finally, a list with the center positions of points of interest can be saved into a script to be scanned automatically (particularly interesting for night shifts).

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For the optimisation of the scanning parameters, *which_distance* takes as inputs the beam energy and pixel size, and returns the critical propagation distance z_c as defined in [5]. *Goto_HA* is used to move automatically to the right *yrot* (y translation under the rotation stage) offset position when performing a half-acquisition scan (allows to almost double the FOV). Outside field of view position in unreachable and messages have been put in place to warn users when the amount of offset is close to the theoretical maximum (45 % of the total number of pixels on the camera across the FOV). For large samples, scans covering multiple vertical positions can be performed, either by using *zseries*, *zscan* or *zhelical* macros. *Zseries* requires, the vertical step (*i.e.*, vertical displacement between 2 successive scans), the number of scans required and the scan name. This macro works well for more advanced users but for more novice ones, *zscan* appears to be less error prone, as the macro requires only the start and end point of the area to scan along the vertical axis and the scan name. It calculates automatically the number of scans required, the displacement and the amount of overlap between the scans. This step can be iterative until a good compromise (number of scans/overlap vs total scan time) is reached. The macro *zhelical* corresponds to helical scanning, which requires the vertical length to cover and the number of turns. While helical scanning is faster on the acquisition side, it is for the moment more complex, thus longer, on the reconstruction side.

Once the scanning is finished, the reconstruction is performed with Nabu [6] through Tomwer [7]. Nabu is the tomography processing software developed at ESRF by the Data Analysis Unit, whilst Tomwer is offering tools to automate acquisition and reconstruction processes for tomography. It contains a library to access each acquisition process individually, GUI and applications to control the main processes (reconstruction, browsing scan and reconstructed volumes, ...) and execute them as a stand-alone application, and an Orange add-on to help users define their own workflow [8].

An example of complete Tomwer workflow is given in Figure 2, where the following widgets are used:

- *scan listener*: is used so that as soon as a scan from the current session is finished, the data are automatically sent to the first processing widget, without human interaction,
- *reduced darks and flats*: the reduced darks are obtained by computing the mean of raw dark frames and the reduced flats are obtained by computing the median of the flats. Those reduced frames will then be used for flat field corrections downstream (for slice and volume reconstruction),
- *default centre of rotation*: used in order to define/search the centre of rotation. The widget contains several algorithms that are better adapted to different types of samples/acquisition,
- *nabu slice reconstruction*: to reconstruct one slice. Several parameters can be tuned, such as Paganin phase retrieval, orientation of the slice, slice index, double flat field correction, ring artefact removal...
- *data viewer* & *volume viewer*: to display the reconstructed slice, and browse the full dataset,
- *scan validator*: displays the last reconstructed slice, if the reconstruction is satisfying, the user can validate the parameters and automatically automatically trigger downstream processing (reconstruction and casting in this example),
- *slurm cluster reconstruction* & *slurm cluster casting*: as the reconstruction and casting are resource intensive, those two operations are performed onto a cluster and not on the local beamline machine. Theses widgets define the cluster resource configuration required,
- *nabu volume reconstruction*: to reconstruct the data,
- *cast volume*: cast the reconstructed volume into a stack of .tiff images (8 bits, 16 bits, 32 bits, or 64 bits), with or without rescaling from percentiles,
- *supervisor*: to follow the status of the jobs submitted to the cluster.

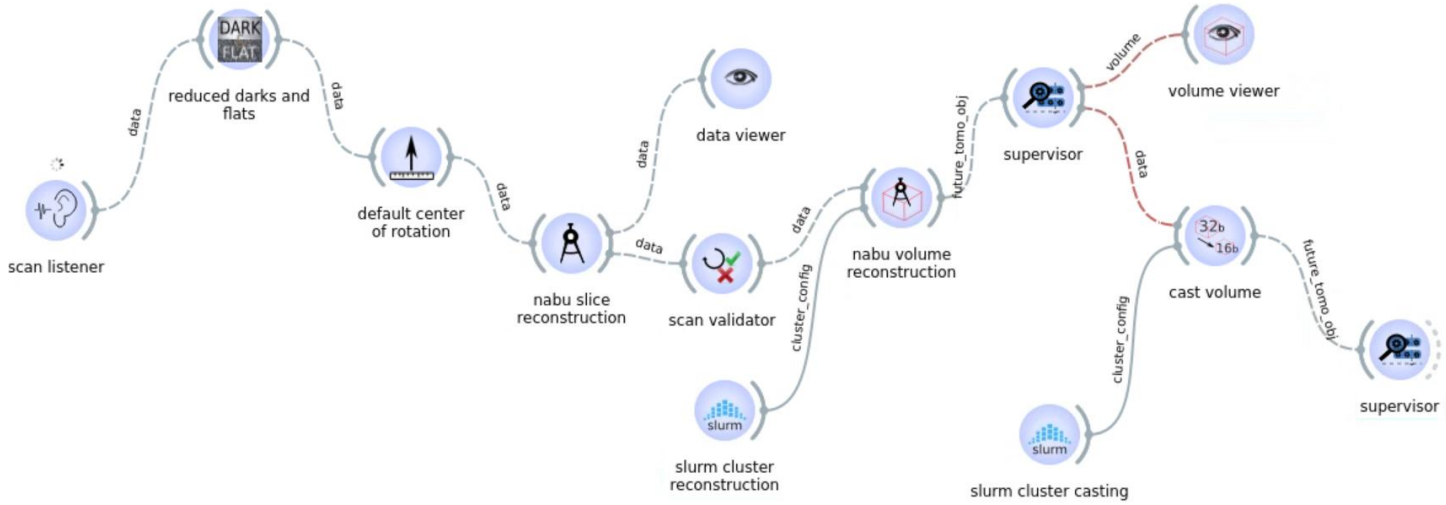

Figure 2: Example of Tomwer workflow

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Overall, this entire workflow can run automatically, *i.e.*, all volume reconstructed and exported as a series of 16 bit .tiff images without user intervention (scan validator can be by-passed if samples are similar). As a result, for simple scans and/or HA scans, users can have all their data reconstructed and cast few minutes after the end of their last scan.

In order to achieve high level of stability and repeatability, procedures had to be put in place for regular assessment of the different elements of the beamline. After each major shut down of the ESRF, the optics need to be realigned onto the X-ray beam. in order for both industrial and academic users to find the beamline in a ready for action state, a restart protocol has been put in place:

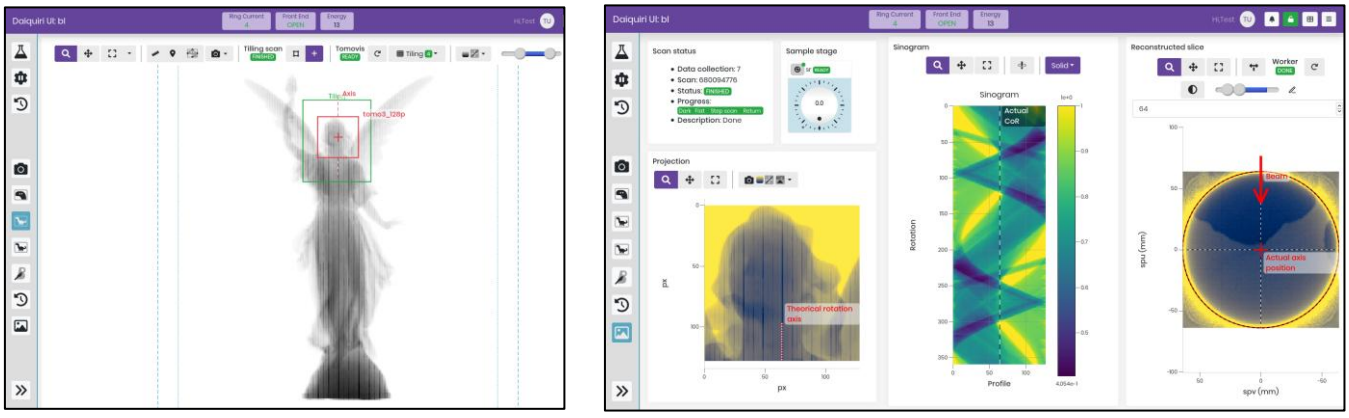
1. First the Dzoom optics is used with its largest pixel (25.5 µm). With a FOV of 52 x 52 mm and both primary and secondary slits fully opened, it is possible to see the beam profile along both horizontal and vertical directions.
2. The optics is then centered onto the maximum of the beam profile in both directions. This operation can be done manually or automatically (automated centering script).
3. The slits (primary and secondary) are then closed to the edges of the FOV, to decrease the amount of scattered radiation. The slits can now be used to align the other optics, as they are also centered onto the beam peak of power.
4. For each optics, at least one set-up is saved at both end of the pixel size range available (for Zoom and Dzoom optics) and two for each objective of the Twinmic optics (one for central beam position (50-150 keV) and one for side beam position (25-30 keV). Those set-ups are being saved in an object called *Multires.* This object saves all motor positions and scan parameters (beamline snapshot) under a friendly name, and allows returning to them easily

For each new set-up required by the user/customer, the parameter of the beamline must be adapted. To save time, the set-up closest to the one required is recalled and as few parameters as possible are adjusted. Once this new set-up is ready, it is saved into *Mutires* so it can be easily called back during the same beamtime or in the future. *Mutires* was developed so that scans with different set-ups (usually using different pixel sizes) can be made successively and easily. With the current format of *Multires*, it takes only few minutes to change from one saved set-up to the next.

Another macro being used is relevant to the scintillator. *Dofocus* runs a focus scan to detect scintillator tilts then provides as an output directly the number of turns for each adjusting screw (one for vertical and one for horizontal tilt) and direction. In terms of processes, routine cleaning of scintillators is important. It appears that scintillator with reflective coatings are much less sensitive to dust and humidity. Another important routine cleaning is linked to the de-darkening of the optics using UV lights. At the moment, the objectives are cleaned when necessary but a more systematic approach based on in-line measurements of the mean intensity in the flat field images is being developed.

2.2 Daiquiri tomo GUI

Daiquiri is a web-based UI framework for control system monitoring and data acquisition. It provides simple, intuitive, and responsive interfaces to control and monitor hardware, launch acquisition sequences, and manage associated metadata. Daiquiri concerns itself only with the UI layer, does not provide a scan engine or controls system but can be easily integrated with existing systems. For tomography applications, Daiquiri is used to perform mosaics of large FOVs in 2D at 0° and 90° so that the centering of samples and selection of ROI is greatly simplified (see Figure 3). The acquisition of those mosaics is continuous (fast tiling radiographic imaging) and thus much faster than the acquisition of a series of successive 2D projections. Specific widgets have been created to allow for fast tiling over an entire sample and subsequent definition of ROIs with sample markers on orthogonal projections.



a) *b)*

Figure 3: Examples of Daiquiri screenshots with a) tiling view of the entire sample with selection of ROI, and b) scan of the selected ROI with corresponding sinogram, and reconstructed slice. The GUI is a much simpler option for a non-expert user to pilot the beamline and perform most of the scanning tasks they require, in a robust, safe, and efficient fashion.

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The main applications for Daiquiri will be for non-expert users and large samples. For non-expert users, Daiquiri provides a GUI that is a simple stand-alone tool to be capable of running their scanning tasks alone in a user-friendly fashion. For samples larger than the FOV of the camera (or complex shaped samples), Daiquiri allows for an easy location of the ROIs within the sample, simple centering and sequential scanning. One such example would be electronics boards and components, where despite the high aspect ratio, customer expect high resolution. High resolution means very limited FOV, usually 1 mm^2; so the identification and centering of the ROI for boards typically of 80mm x 50 mm x 2 mm can sometimes take up to 30 min, due to the large number of features with repetitive geometries (soldering balls, chips…). Daiquiri provides simple visual solutions to complex centering problems and alignment in 3D.

2.3 Sample changer

The BM05 robotic sample changer is an equipment designed to automatically change samples from its sample storage shelves to the tomograph. It allows users/operators to program and automatise a series of microtomographic scans, without entering the experimental hutch. The robot arm is a commercial TX60 L CS8C provided by the company Stäubli [9] and the whole ensemble has been in-house designed and assembled in collaboration with 6TEC company.

The robotic arm uses a laser to learn the target position onto the base plate on the tomograph. This operation has to be performed each time the sample changer is disconnected and moved away from the tomograph (for in situ experiment for example). The laser, alongside the kinematic base, ensure accurate positioning/repositioning of the samples, even at highest resolution (0.36 µm pixel size). Using the sample changer requires the following steps, detailed below:

- Sample mounting on magnetic bases
- Organize samples on sample shelves
- Align samples within the FOV
- Record sample positions within FOV (*sx*, *sy*, and *sz*)
- Write a macro with every scan required for each sample, could be at multiple resolution (as long as the set-up is saved and can be recalled by *Multires*), multiple ROI per sample, …

First the samples are mounted onto the magnetic base available on the beamline. One hundred bases are available and can be used by the sample changer but also by users, directly on the tomograph. Then the bases are physically put on the sample changer shelves, at labelled positions. Three shelves are available, that can host a total of 45 samples, of maximal dimensions of 100 x 60 x 150 mm and maximum weight of 3 kg. Both physical and digital record sheets have been created to enter the correspondence between sample name and labelled position on the sample shelves. It is not necessary to define the sample name in the sample changer acquisition system, as the naming of the scans is done inside a Python script that gathers all the information relevant to the sample. Then the samples to scan are loaded one by one and aligned within the FOV of the required optics. The sample positions are recorded and put inside a macro. By using a macro to run the scanning of each samples, it becomes simple to make custom made scans, *e.g.*, the same sample position can be scanned at different pixel sizes very easily. The main interest of the sample changer is to run samples overnight, to maximise usage of beamtime.

3 Conclusion

Synchrotron tomography provides unique characteristics in terms of scanning speed and resolution. However, the complexity level in running and maintaining the performance of a synchrotron beamline is very high. To attract new academic users, the beamlines need to be more user-friendly, robust and easy to use. To attract industrial users, standards and quality control play an important role. In both cases, some of the solution will be brought by automatisation and procedures. Automatisation make sure that some operations can be performed automatically in a minimum amount of time, and procedures are put in place so that this automation is reliable. Overall, improvements made on BM05 with the implementation of automated macros and routine procedures lead to increase stability, reliability, ease of operation, and throughput.

The ways to improve a beamline in terms of performance, smoothness of operation, and reliability can be divided into three aspects: hardware, software, and processes. Current and future developments will focus on:

- hardware: testing of new cameras, scintillators and optic systems
- software: distortion maps for each objective (to improve the quality of reconstructed data), automatic sample centering for easy cases, automated calculation of beam energy based on beamline and attenuator configuration (based on OrAnge SYnchrotron Suite OASYS [10])
- procedures: full review of operational procedures for industrial tomography, improved software documentation for users

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