

IMX Beamline: X-ray Imaging

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Gabriel Schubert R.C.,	gabriel.costa@lnls.br	1142
Gustavo J. Q. Vasconcelos,	gustavo.vasconcelos@lnls.br	3542
Carlos Sato B. Dias	carlos.sato@lnls.br	2517
Nathaly L. Archilha,	nathaly.archilha@lnls.br	1043
Eduardo X. Miqueles ,	eduardo.miqueles@lnls.br	1043
Francis P. O'Dowd,	francis.odowd@lnls.br	5078

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A K-Edge angles for multilayer and Si crystals.

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1 Introduction

The Brazilian National Light Source (Laboratório Nacional de Luz Síncrotron - LNLS), was established in 1986 as a research institute funded by CNPq, the National Research Council of the Ministry of Science and Technology (MCTI). The choice of a synchrotron light source, as the first modern National Laboratory in Brazil, arose from a perception of the need to develop accelerator technologies, basic experimental research and applied materials research as well as a new model of scientific organization in the country.

The synchrotron facility was built in the intervening years and was finally inaugurated in 1997. It is an open facility that serves the scientific and business community across the country and abroad and is collocated along with three other national laboratories - Brazilian Bioetanol Science and Technology (CTBE), Brazilian Biosciences National Laboratory (LNBio) and Brazilian Nanotechnology National Laboratory (LNNano). The facilities are annually used by about 2,700 Brazilian and foreign researchers, on a “free to use” basis, committed to over 500 studies that result in approximately 250 articles published in scientific journals.

The LNLS beamlines operate 24 hours a day in three shifts of 8 hours, with no beam provided during the weekends and the majority of Mondays. The 18 beamlines, each dedicate about 425 shifts per year to peer-reviewed projects. During the year, two long shut-downs are scheduled: 4 weeks in summer and 2 weeks in winter. Other breaks in the operation are for machine-dedicated runs and maintenance days, usually occurring once a month.

During your experiment, a scientist familiar with the beamline will be there to guide you. This person is known as the Local Contact. His/her task is to prepare the beamline and help you to begin your experiment. In case of major difficulty, and if your local contact is not present on the beamline, you should contact the Emergency Number (686), who will decide what kind of action can be taken.

1.1 Policies

Users are required to acknowledge the use of LNLS facilities in any publications and to inform the Laboratory about any publications, thesis and other published materials. Also, users should cooperate by supplying this information upon request. If you publish data

collected at IMX, please acknowledge the use of the beamline in the Methods and Acknowledgements sections and cite the reference publications.

After finishing the research project, we highly recommended all users to fill the Feedback on infrastructure and services provided at the SAU Online and Experimental reports.

1.2 Tomography

Tomography is a non-invasive imaging technique that allows to examine slices of a sample without damaging it. While radiography provides an image from a single orientation of the sample, tomography provides many images of the sample from different orientations, resulting in a set of projections or sinograms. Essentially, each sinogram column corresponds to the X-ray projection at one angle. This data can then be reconstructed by basically solving the inverse Radon transformation.

In our case, filtered back projection is used to reconstruct 3D images from a series of 2D projections. The projection values are smeared back across the 2D projections and integrated across all angles. To reduce blurring effects, the images are filtered in Fourier space before being back projected.

Phase Contrast – Propagation Based

Similar to tomography, this method involves placing the detector some distance from the sample, so that the radiation refracted from the sample can interfere with the unchanged beam. Given the high degree of coherence available in synchrotron radiation, interference patterns or Fresnel fringes can be observed some distance away from the sample. Using this technique allows us to enhance the contrast observed in absorption images or separate entirely the phase (phase retrieval) and attenuation components. This method is particularly useful when investigating light materials or biological samples or even composites made from similar materials.

Other techniques currently under development include Phase Contrast – Talbot Interferometry, Differential Absorption Tomography and Missing-Wedge Tomography.

1.3 Arrival at Beamline IMX

The LNLS website has the most up-to-date and relevant information for all the preliminaries regarding a visit to the laboratory, including accommodation <http://lnls.cnpem.br/>. After passing through the Users Support Office (SAU), the user can access the experimental hall, using their LNLS badge and dosimeter. Figure 1 below shows the location of imaging beamline IMX.

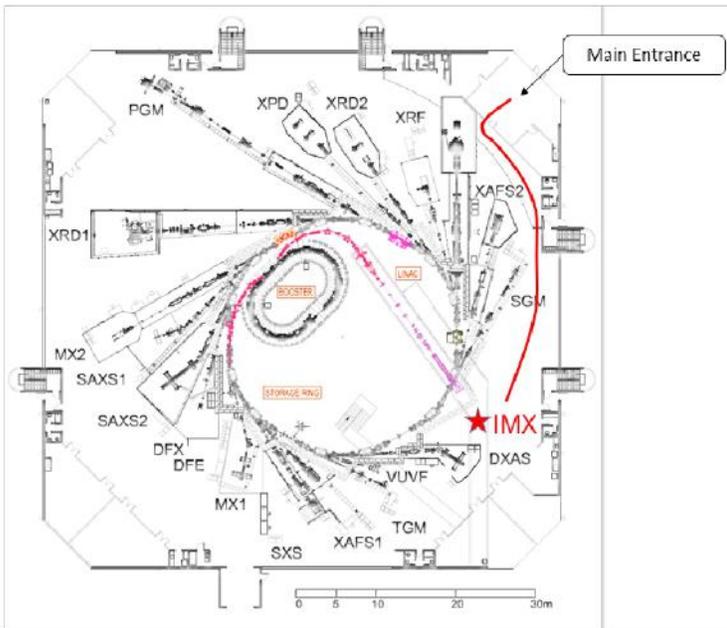


Figure 1: IMX Beamline location

1.4 Safety

The safety objectives is guarantee the life and a safe environment for work. The primary control for workers protection will be engineering controls such as exhaust ventilation and flow limiting devise such as reduced flow orifices. The engineering controls will be evaluated on a case-by-case basis. We expect that the engineering controls will limit the exposure of toxic gases to workers for 99% of all situations. In the 1% of cases where engineering controls cannot ensure that the concentration of the toxic gas being emitted at the exhaust stack does not exceed the IDLH concentration, the most stringent engineering controls will be used as well as administrative controls such as limiting access to the roof.

The users are requested to inform the local contact of any risky

materials. Usually, before an experiment takes places, all samples have to be reported via the Safety of Samples, Standards and Routines A Form to the safety group. Only after validation by the safety group, the experiment may be perform.

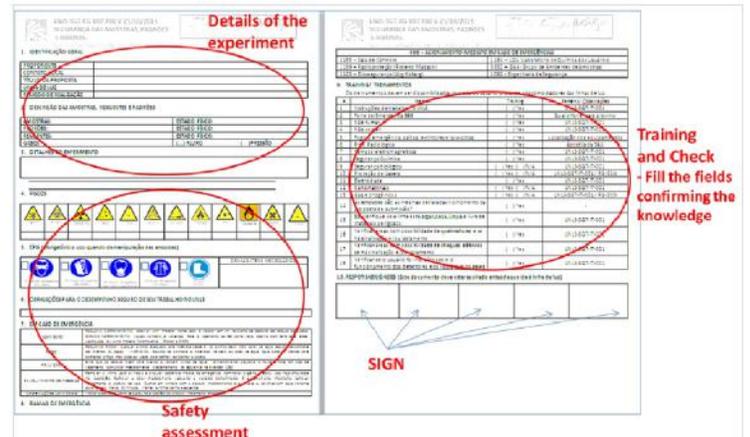


Figure 2: Safety of Samples, Standards and Routines Safety Form

When the user arrives, the staff member (or local contact) will fill the fields of the safety form with user, informing the necessary points of safety. In case of any doubt, access the LNLS safety training procedures.

At the beamline, if the users are not sure of the risk that an operation could entail, please consult with the local contact beforehand.

2 Technical Information

The imaging beamline, IMX, at LNLS has an electron source size of $391 \mu\text{m} \times 97 \mu\text{m}$ and beam divergence of $808 \mu\text{rad} \times 26 \mu\text{rad}$. Synchrotron radiation is extracted from bending magnet D6, which has a magnetic field of 1.67 T and bending radius of 2.736m.

Energy Range	5 keV to 25 keV - Pink Beam 5 keV to 14 keV - Multilayer DMM 5 keV to 14 keV - Si(111) DCM
Energy Resolution	Si(111) 1.3×10^{-4} Ru/B4C ML 1.4×10^{-2} Pink Beam
Source	$391 \mu\text{m} \times 97 \mu\text{m}$ (HxV) from Bending Magnet 1.67 T

The monochromator is 12 m and the sample is 17 m downstream from the source. This beamline can operate in either white beam or monochromatic beam. Monochromator elements are Si(111) and a Ru/B4C Multilayer pair. Both elements are water cooled. Monochromator elements can be removed from the beam to allow white light to enter the hutch. White beam energy spectrum ranges from 5 keV to 14 keV, with a photon flux at the sample position of approx. 10^{15} photons/s.

Flux density at the sample

8.61×10^{13} Ph/s/mm² for 100 mA stored current - Pink Beam
 1.22×10^{10} Ph/s/mm² @ 8 keV for 100 mA stored current
 Ru/B4C 1.84×10^8 Ph/s/mm² @ 8 keV for 100 mA stored current
 Si(111)

Beam size at the sample

13 mm x 10 mm (HxV) - Pink Beam
 13 mm x 4 mm (HxV) - ML/Si(111)

Optics

Double Multilayer Monochromator - Ru/B4C Double Crystal Monochromator - Si(111)

Image Detection

Optique Peter Low-Dose microscope with PCO 2000 CCD camera
 Optique Peter High-Dose microscope with PCO 2000 CCD camera

3 Beamline Description

A description of the beamline is presented in Figure 3

Experimental Hutch : The sample is mounted on a high precision stage with 6 degrees of freedom including two linear stages

with less than $1 \mu\text{m}$ resolution for positioning the sample in the detector field of view.

Filter : Adjusts the synchrotron energy distribution of 4 ~ 20 keV by effectively blocking low energy part of X-rays to reduce the heat load on the sample by using four aluminum sheets.

Shutter : It turns synchrotron radiation on and off to prevent samples from excessive exposure to synchrotron radiation by controlling the exposure time. It can also control the radiation dose necessary for the experiment.

Ion Chamber : The air-ionizing chamber measures the photon flux to estimate the radiation doses absorbed by samples.

Slits : Properly cuts off the synchrotron radiation size in the line with a size to fit to the region of interest in the sample and the scintillator.

A gama shutter is located inside the storage ring and can be shut to allow access to the hutches of the beamline. Typically users will not need to access the optical hutch. Also three vacuum valves are located on the beamline: i) just inside the storage ring wall, ii) before the monochromator and iii) after the monochromator. More details on arming the hutch and preparing for beam is presents in the section of arming the hutches.

At the entrance to the optics hutch the beam is first conditioned by white beam slits, before passing through a water-cooled Beryllium window ($125 \mu\text{m}$ thick) before the monochromator. Following this, the beam passes through a small nitrogen filled ion chamber, then the final Beryllium window, which separates the vacuum from the air in the experimental hutch. The fast shutter controls the dosage on the sample, before the beam passes through a small vacuum section, provided by two Kapton windows ($25 \mu\text{m}$ thick). A set of carefully optimised filters are available, which can be inserted into the beam path to remove low energies. These are particularly useful when imaging heavier or fragile samples where the lower energies either significantly damage the sample or result in beam hardening. The set consists of 4 highly polished Si filters of 200 and $350 \mu\text{m}$ thickness that can be combined to offset the average energy. Finally, a set of high precision slits defines the beam profile just before the sample.

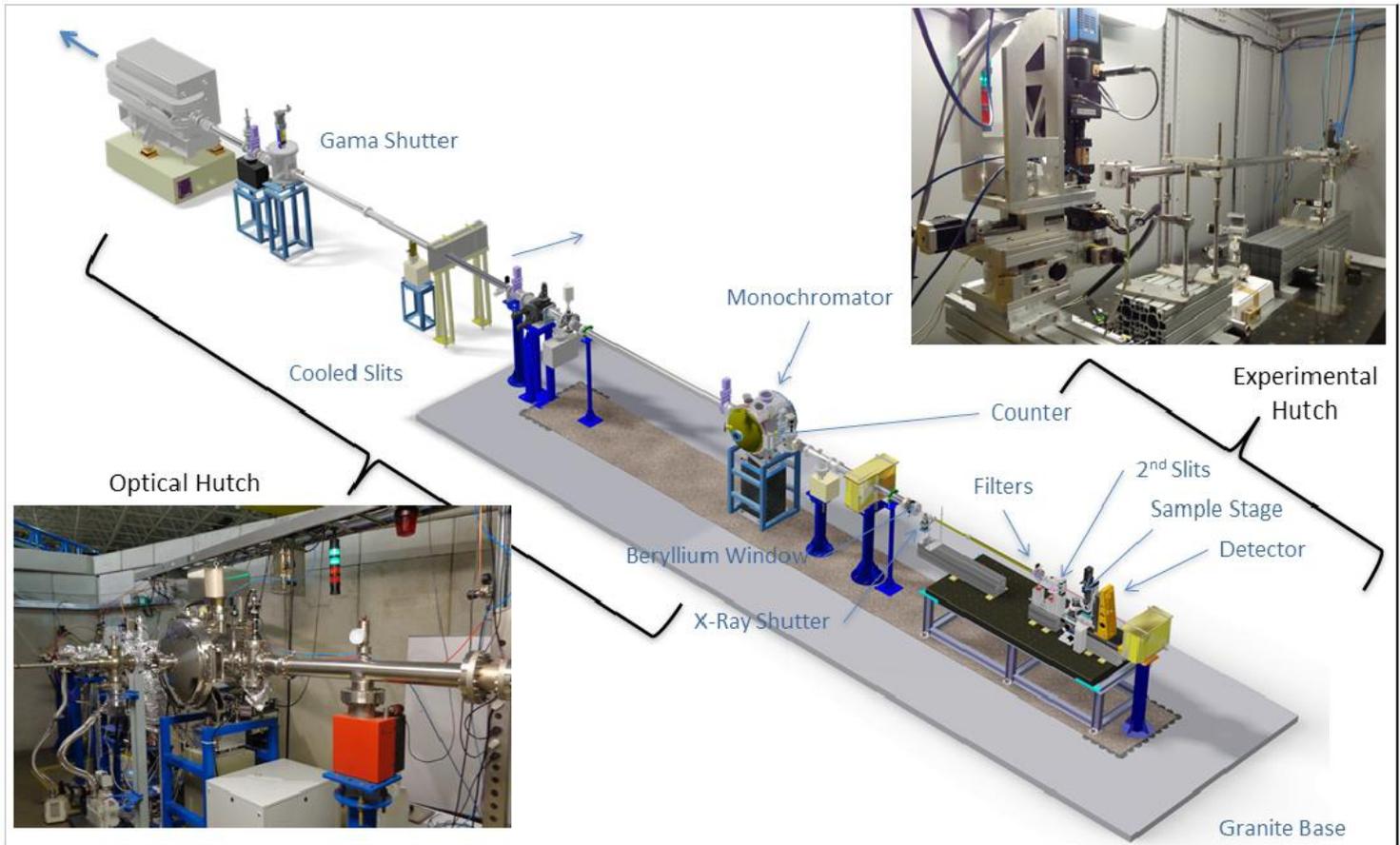


Figure 3: Beamline description

The sample stage is located a few centimeters downstream of this set of slits. This stage allows for 2-dimensional translation (in the plane perpendicular to x-ray beam propagation) with sub-0.1 micron precision, to allow positioning of the sample within the x-ray beam, or to allow tiling of images. An air-bearing rotation stage, used for tomography scans, sits on the translation stage. Two high precision linear stages, mounted transversely to each other, allowing positioning of the sample over the axis of rotation. A magnetic sample mount is placed on top of the rotation stage, to locate the sample on the stage.

After passing through the sample, the X-rays pass through a thin vitrous carbon glass cover to enter a light-tight camera box. The x-rays reach a scintillator, which produces visible light; the local contact will select from one of 6 available scintillators; scintillator materials include Tb:LSO, LuAG, GGG, and Yag:Ce, of varying

thicknesses, each optimized for work at different resolutions. Directly behind the scintillator is a mirror, set at a 45 degree angle. A turret containing long working distance lenses can then be used to image the scintillator onto a pco.2000 CCD camera. The objective is mounted on a stage which controls the image focus. The image recorded by the camera corresponds to a parallel projection of the sample onto the scintillator by the x-ray beam. In tomographic scans, a series of projection images are taken while the sample is usually rotated 180 degrees. The entire camera box move on two stages, which allows the sample-to-detector distance to be varied from a minimum of approximately 1 mm to a maximum of 300 mm and height to be adjusted given the monochromatic beam offset.

Please note the coordinate system in use at the beamline:

- X: transverse to beam direction;
- Y: Vertical direction and;

- Z: Beam direction

3.1 Endstations

3.1.1 Microscope

Optique Peter have designed a novel modular based indirect detector for X-Ray micro-imaging. It can be adapted for different cameras, i.e. different sensor sizes and can be tailored to work either with monochromatic illumination and the correspondingly lower absorbed dose or with intense white beam irradiation. In order to allow for a high level of compatibility, a common camera support represents the backbone of the microscope. It consists of a tube lens, a motorized camera rotation, a camera mount and a flexible interface system. A so-called low-dose head or high-dose head can be mounted to this common support. The difference between the two being the removal of the microscope objective from the x-ray path.

The camera head and the objective head can be motorized. The objective head can be equipped with 3 different high-quality objectives, allowing quick change between different field of views and spatial resolution.

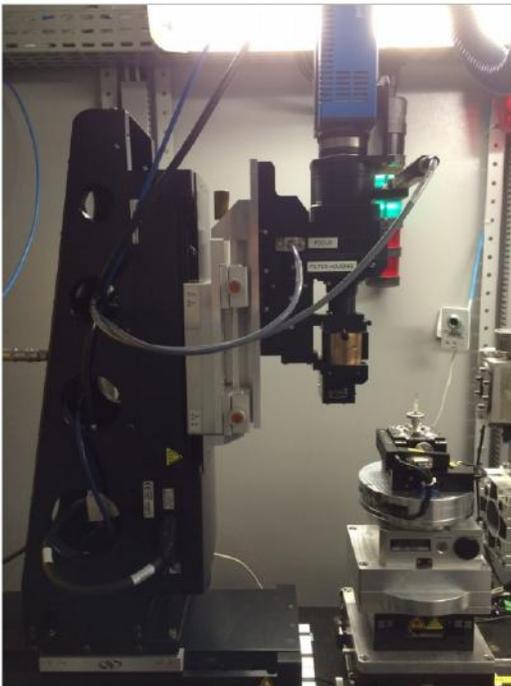


Figure 4: IMX Detection System

3.1.2 Camera

The microscope is currently used in combination with the pco.2000 camera. The PCO.2000 is a high resolution 14-bit CCD cooled camera. This camera has a sensor size of 2048 × 2048 pixels, where each pixel is 7.4 μm. For the low-dose configuration, this results in a FOV of 3.8 mm × 3.8 mm for the 4x objective; 1.52 mm × 1.52 mm for the 10x objective and 0.76 mm × 0.76 mm for the 20x objective. In high-dose configuration a 5x objective can be used to obtain a FOV of 3.4 mm × 3.4 mm and a 10x objective can achieve 1.7 mm × 1.7 mm.

- Monochromatic characteristics for PCO 2000 Camera (2048 × 2048 pixels, 7.4 μm × 7.4 μm):

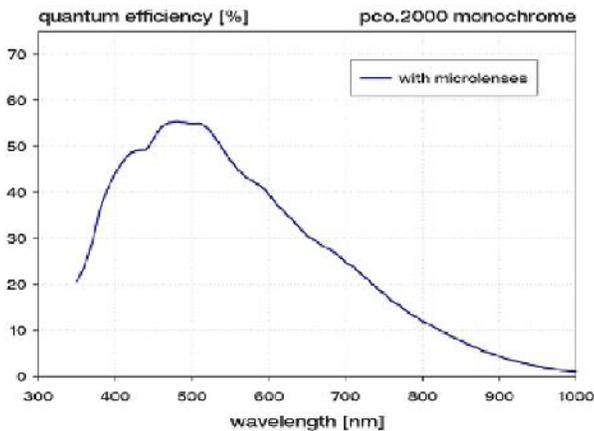
Objective	Pixel Size (μm)	Hor.Fov (mm)	Vert.Fov (mm)	Depth of focus ±	Resolution Limit
2x	3.7	7.6	7.6	66μm	4.2μm
4x	1.9	3.8	3.8	17μm	2.1μm
10x	0.74	1.52	1.52	2.6 μm	0.84 μm
20x	0.37	0.76	0.76	0.74 μm	0.45 μm

- White Beam characteristics for PCO 2000 Camera (2048 × 2048 pixels, 7.4 μm × 7.4 μm):

Objective	Pixel Size (μm)	Hor.Fov (mm)	Vert.Fov (mm)	Depth of focus ±	Resolution Limit
5x	1.64	3.4	3.4	19μm	2.4μm
10x	0.82	1.7	1.7	4.7μm	1.2μm

The camera has a quantum efficiency of 55% at 500 nm, as shown below, Figure 4, and has a full well capacity of 40,000. Imaging frequency at full resolution is 14.7 fps, however binning modes in the horizontal and vertical are available.

A dedicated machine running Windows OS controls the pco.2000 camera through a GigE interface. The machine has two network boards to handle high data throughput during scans. A dedicated TOE (TCP/IP Offload Engine) network board receives data directly from the camera, and a second network card sends data to the data storage location. Once the data reaches the storage, other computers can remotely access it to process or analyze information. In the data route from the camera to the storage, the network configuration relies on big package transmission to minimize package loss and



network latency. Package size and number of coalescence buffers are high, and all the network switches between the camera and the storage have QoS (Quality of Service) priority configuration. The storage is a GPFS file system with the purpose of providing better cost-effective scalability. With such configurations, the data transfer rate reaches 100 MB/s, or around 12 fps at full resolution. On the Camera Control application, a queue system is included to account for any additional latency on the network.

In this implementation, a LabVIEW code configures the camera, translating PVs into camera inputs, and writes binary projection data to the storage location. Unnecessary interruptions and EPICS Client PV checks are disabled during tomography and re-enabled afterward. As a way to avoid unnecessary file conversion tasks, external scripts access the binary files from the storage location to convert data to HDF5, TIFF or other image format requested. For the purpose of tomography reconstruction, all images are stacked into a single HDF5 format image. In this way, it is possible to retrieve each projection for the various angles and extract the sinogram directly by changing the stack's cutting plane dimension.

Microscopes can be changed for specific requirements or experiments but can be done so only by IMX beamline staff

3.1.3 Scintillators

A scintillator is a material that exhibits scintillation — the property of luminescence when excited by ionizing radiation. Some of the

basic requirements for high-resolution X-Ray imaging scintillators are:

- High X-Ray absorption to maximize the X-ray stopping power.
- High conversion efficiency of x-rays to visible light, emission wavelength well matched to the CCD readout (490-560 nm), low afterglow and high linearity of the light output with the X-ray flux.
- High transmittance and no scattering – excellent optical properties.

Scintillator options	
Tb:LSO, ϕ 10mm, 8 μ m	high resolution
LuAg:Ce, ϕ 10mm, 50 μ m	high flux
LuAg:Ce, ϕ 15mm, 5 μ m	high resolution, large fov
Yag:Ce, ϕ 8mm, 5 μ m	low/medium flux
Yag:Ce, 9x9mm, 50 μ m	high flux
GGG, 10x10mm, 10 μ m	low/medium flux

Scintillators can be changed for specific requirements or experiments, but again, can be done so only by IMX beamline staff

3.2 Additional Diagnostics

Beam diagnostics can be measured at the output of the monochromator, the entrance to the experimental hutch, before the sample and the imaging detector itself. At the output of the monochromator are two fluorescence screens which can be placed into the beampath. One set of screens, for white and monochromatic beam, installed inside the monochromator can be manually positioned to show the beam position. For white beam the lower screen should be positioned at 46 mm, and for monochromatic beam the top screen should be positioned between 36 and 41 mm. IMAGE

At the entrance to the experimental hutch is an ion chamber. This chamber is positioned before the fast-shutter so is continuously exposed to the incoming radiation. Voltage is supplied (400V) from a high voltage power supply and the measurement is amplified using a Stanford Pre-Amplifier. The signal is passed to the NI-PXI and can be readout from the PV.

After the last set of slits, a Cyberstar photomultiplier device is mounted which gives a measure of the beam flux entering the sample. Data Acquisition Architecture

The LNLS X-Ray Imaging Beamline (IMX) uses a National Instruments PXI-6602 timing board attached to an NI PXI-1045 chassis to read digital counters and trigger devices during scans. A Huber 409 rotation stage performs the sample rotation during tomography. The scan points are programmed directly on Galil DMC-4183 motion controllers as a function of parameters passed from EPICS PV's to reduce latency between scan points and enable quick tomography. The controller sends feedback through the I/O interface on trip-point arrival and transmits the present motion status, enabling hardware synchronization between motors and scan devices. A LabVIEW VI running on a dedicated Windows Machine controls a pco.2000 camera, which is currently the main detector at IMX Beamline. The user interface screens run from a workstation on CS-Studio environment under Linux Red Hat operational system. CS-Studio inputs integrate to EPICS via Py4Syn scripts to run scan routines and set up experiments.

Upon request, several laboratories are available for users on site.
Chemistry Support Laboratory - Scientist in charge: Simone (Rama-
mal: 1184)

Outside working hours (from 8h00 to 17h00, from Monday to Friday) the use of the LNLS Chemistry Laboratory should be specified in the Chemistry Laboratory form.

4 Sample Setup

The first consideration is sample size. Please see camera specifications section above for tables showing the field of view for each lens/camera combination. Ideally, the sample should remain within the FOV for all angles, thus the size of the sample is limited by the chosen objective and resolution.

For special cases, the sample is wider than the field of view, "local tomography" can be used-in this mode, the sample is mounted such that the sub-region of interest remains in the field of view, even though parts of the sample may leave and enter the field of view during sample rotation. While local tomography does yield some artefacts, results are surprisingly good.

It is also possible to run tomography scans through 360 degrees. In this case, the FOV is approximately doubled (some overlap is required). The centre of rotation can be positioned on the right hand side of the image and a full tomography can be acquired in which half the sample will be imaged in half of the scan. This does require some changes to the reconstruction parameters as well as a longer acquisition time which will be discussed in more detail later and must be requested with your local contact before arriving at the LNLS.

Another option is to use vertical and horizontal tiling. Thus it is possible, in theory at least, to collect images of a sample that is smaller than the full travel ranges of these stages. In reality, however, transmission is major problem on large samples as is the accuracy of the stages. Coupled with this, lens distortion at the edges of the image can cause imperfect stitching which leads to artefacts in the tomographic reconstruction because a single centre of rotation cannot be found that gives a suitable reconstruction for the entire tiled image. This method can also result in extremely large datasets that can be difficult to reconstruct and process.

A second consideration is sample shape. Cylindrical samples are preferable to square samples, because the sample thickness for the transmitted x-rays remains approximately constant as they rotate. Because optimum imaging is obtained for approximately 30% x-ray transmission, it is ideal if this level of transmission is constant through a tomographic scan as the sample is rotated.

A third consideration is the sample container. It is desirable to have a minimal contribution from any mounting or contain-

ment materials—thus, these should be eliminated or made as thin as possible. Highly absorbing containers are especially problematic—especially if their absorption is higher than that of the sample. Note that any object (wire, screw, etc) that crosses vertically through the field of view will cause problems. Ideally, containers should fit within the field of view, and should be uniform to reduce any artifacts they may contribute.

In many cases, it is desirable to place the detector very close to the sample (on the order of a millimetre) to reduce the phase contrast contribution to the image. In these cases, it is critical that the above advice on sample shape and on containers be followed, so that the sample can be rotated despite the short sample-detector distance.

4.1 Sample Preparation and Handling

Sample preparation should be performed at the designated user's laboratory (LQU) under the supervision of Simone Betim (simone.betim@lnls.br, ramal:1184). Notice that the LQU is a shared facility under an independent administration, and that it is your responsibility to coordinate with the beamline staff and LQU staff any special need regarding sample preparation.

Sample mounting should be performed on the work bench in the designated area. Safety glasses should be worn when working in this area.

In any case, all users should first report at the beamline and then coordinate with the beamline staff the sample preparation and sample mounting.

4.2 Sample Mounting

The sample is mounted on a kinematic mount that is, in turn, attached to the top of the rotation stage by a magnet. Several sample stages are available on the beamline and best shape/size mount should be chosen for the sample.

Samples should be rigidly mounted, to avoid unwanted sample motion during a scan; if a sample moves during a scan, **the reconstruction will not work**. Options available at the beamline for mounting the object to the sample stage include:

- drill chucks;

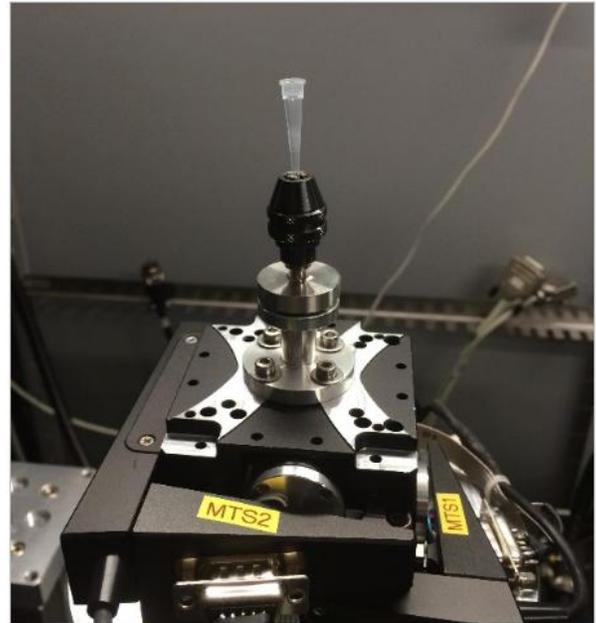


Figure 5: Kinematic Sample Mount

- double-sided tape (put it on top of a mounting post, and stick sample to it)
- kapton tape (tape sample to a post or other holder)
- styrofoam (hollow out a hole between two pieces of styrofoam, and tape them around the sample)
- plasticine/clay (mold it around the base of your sample)
- wax (melt it, put sample in, let it set)
- plastic or kapton tubing (jam sample into it, or use foam or plastic wrap to pad it, or washers or o-rings to hold it in place)
- pipette tips

4.3 Sample Aligning

Before the Align Sample script can be executed, it is necessary to ensure the sample, or some part of it, is within the field of view at 0°, 90° and 180° (270° if 360° scan is used). The two stages, mounted on top of the rotation stage, MTS1 and MTS2, can be manipulated such that the sample (or, in the case of local tomography, the center of the region of interest), is located within the fov of the detector. The reason for this is that a centred sample will remain in the field

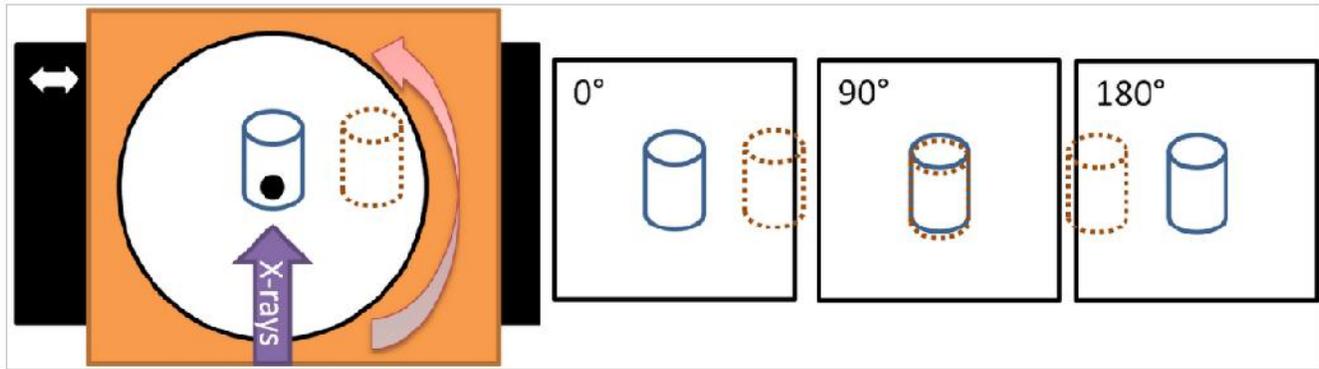


Figure 6: Correct and incorrect sample centering

of view throughout the rotation, while an un-centred sample may leave the field of view (see diagram above - the blue cylinder is centred on the axis of rotation, while the dotted red cylinder is not; the dotted cylinder enters and leaves the field of view as the stage rotates).

To begin this process, you can use the laser in the experimental hutch to 'locate' the sample in relation to the x-ray beam. Simply place the mirror in its mount, before the last set of slits and turn on the laser. The laser beam simulates the path of the x-ray beam and the sample position can be adjusted manually. Remember to remove the laser mirror before arming the hutch. Using x-rays, image the sample position at 0° , 90° , and 180° (if 360° scan is used, be sure to image at 270° as well). At this point you can image the sample using a low exposure time so as to speed up the process. Except for local tomography, the idea is to image the silhouette of the sample, so as to be able to centre it in the image. If the sample is outside the field of view, adjust the MTS1 and MTS2 stages accordingly, using the following guide:

Motor directions	Angle
MTS2: + ← - →	0°
MTS1: - ← + →	90°
MTS2: - ← + →	180°
MTS1: + ← - →	270°

1. Begin at 0° and take an image. If aligned with the laser, the sample should be in view. It may be necessary to move the MTS2 motor to ensure the sample (or at least some part of it) is within the fov.

2. Rotate to 180° and take another image. If the sample is either to the right or left move the MTS2 stage in the appropriate direction (see table above). However, note that moving the MTS2 stage will affect the 0° image. Again adjust until the sample is within the fov.
3. Return to 0° and check the new position. Continue this process in an iterative process until the sample remains within the fov at both 0° and 180° . It may also be necessary to move the Sample X stage, if the sample lines up on the same side at 0° and 180° .
4. For a 180° scan, the 90° position is independent and can be found simply by moving the MTS1 stage until the sample is within the fov.
5. For a 360° scan, it is necessary to check 90° and 270° and iteratively adjust the MTS1 stage until the sample remains within the fov at both these angles. Adjusting the 90° and 270° should not change your previous alignment, however, it may be necessary to move the SampleX stage during this alignment, therefore check 0° and 180° once again.
6. Note, if running a full tomography (360° for larger samples) complete this process first before shifting the rotation axis to the right hand side of the image using the SampleX stage. Note the distance the rotation axis was shifted!
7. In order not to 'lose' the sample during these alignment steps, it is recommended to move all stages in small steps <0.5 mm or smaller depending on the objective.

4.4 Sample Aligning

This is an automated script to precisely align (within one pixel) the sample onto the rotation axis. In order for this script to function correctly, the sample must remain fully within the fov at 0 and 180. The SampleX stage will be positioned automatically in the best location.

4.5 Advanced alignment and optimization

There are other alignment procedures that are not available to the user and should only be done by an IMX staff or under supervision

4.5.1 Sample Focus

The objective of the lens may be focused at any stage before the tomography scan, however, it is recommended to run this step as soon as the sample is in view as it will affect the alignment scripts. It is possible to focus on the sample using a python script by selecting the distance over which the objective lens can be moved and the number of images which should be acquired within this distance. The contrast levels of each image is calculated, with the highest contrast providing the location of best focus. The details for calling the script are shown in the software section.

4.5.2 Adjust Sample-Detector Distance

The distance between the sample and detector has a strong influence on the observed image. This is due to the increase in the phase contrast contribution with increasing distance. The optimum distance for a particular application often must be found by trial and error. We note that phase contrast effects begin to appear even when the sample-detector distance is only a few millimetres.

The following papers may be helpful in understanding phase contrast tomography and in deciding your sample-detector distance:

1. Phase contrast tomography: An alternative approach. Groso, A., Stampanoni, M., Abela, R., Schneider, P., Linga, S., Muller, R. (2006). Applied Physics Letters, 88(21).
2. Implementation of a fast method for high resolution phase contrast tomography. Groso, a, Abela, R., Stampanoni, M. (2006). Optics express, 14(18), 8103-10.

3. ANKAphase: software for single-distance phase retrieval from inline X-ray phase-contrast radiographs. Weitkamp, T., Haas, D., Wegrzynek, D., Rack, A. (2011). Journal of synchrotron radiation, 18(Pt 4), 617-29.
4. Optimization of phase contrast imaging using hard x rays, Zabler, S., Cloetens, P., Baruchel, J., Schlenker, M., Dyck, V., Gureyev, R. (2005). 1-7.

If the detector is moved, it is essential that the camera rotation axis is realigned to the sample rotation axis. To do this a script, Camera Alignment, is available. This script will remove the sample from the FOV, close the fine alignment slits and adjust the rotation angle of the camera accordingly. It is highly recommended to run this script twice, once for a wide range (0.1 mm to -0.1 mm) and afterwards with a narrow range (0.01 mm to -0.01 mm). This will ensure that the rotation axis of the sample will align to a single column of pixels of the detector and simplify reconstruction. The details needed to call this script are provided in the software section below.

5 Hutch Procedures

The IMX beamline consists of two hutches: an Optical Hutch and Experimental Hutch, as shown below in Figure 7. Users will be shown on-site how to arm the hutches, open the valves and shutter and deliver beam to the sample. In order to allow beam into the beamline, both hutches have to be armed. For completeness the routine is provided below.

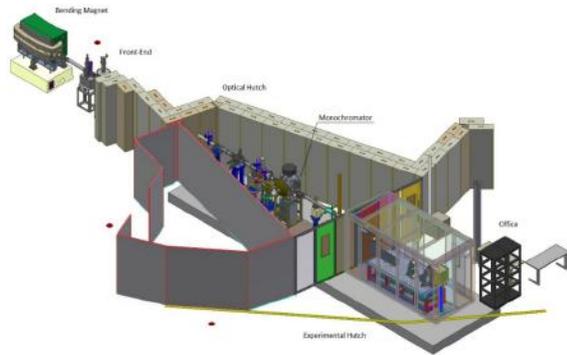


Figure 7: IMX Optical and Experimental Hutches

5.1 Arming the Hutches

To arm the optical hutch, first ensure the hutch is empty by conducting a thorough search. Close the door, careful no do not slam the door. Press the lit 'green' button to secure the hutch. The beacon inside the hutch will flash and an alarm will sound for 15 seconds. The button on the door will now turn 'red' and the hutch is secure. It is necessary to secure the optical hutch before the experimental hutch can be armed, see Figure 8.

There is an Emergency Switch available inside the hutch door – simply PUSH to kill the beam in the hutch.

To arm the experimental hutch insert the Master Control Key into the interlock control box, quarter turn and remove. After this you have approximately 15 seconds to leave the hutch and close the door. Once closed, press the lit 'green' button to secure the hutch. If the door isn't fully closed, the hutch will not arm. You can use this 15 seconds to try to squeeze the doors together, otherwise,

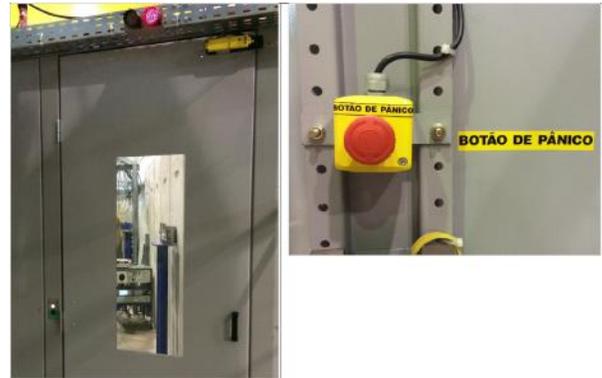


Figure 8: Optical Hutch Door and Emergency Switch

you will have to re-enter the hutch and being the procedure over. Once both hutches are armed, insert the master control key into the control panel. Note all four keys must be present and 'activated' to provide beam in the hutch.



Figure 9: Experimental Hutch Door and Interlock Control Box

Whenever it is necessary to enter either of the hutches, remove a key from the control panel to ensure beam cannot be activated.

DO NOT REMOVE THE KEYS FROM THE BEAM-LINE!

5.2 Opening the Hutches

To open any of the hutches, first close the Gama shutter, if open. To do this simply press the 'OBTURADOR FEIXE BRANCO' switch

on the Interlock Control Panel, wait for the led to go red and remove the Master Control Key.

Approach the experimental hutch door and press on the 'lit' button to allow access to the hutch - Figure 10. The hutch is now unlocked, and you can slide open the doors. The experimental hutch has to be opened before the optical hutch can be accessed in the same manner. Note, it may take some seconds for the interlock to release the hutch door.

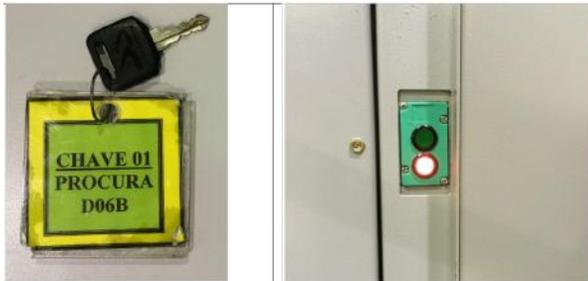


Figure 10: Master Control Key and Hutch Switch

5.3 Opening and Closing Shutters

A series of shielding, shutters, and interlocks protect people from exposure to radiation. Two personal safety shutters are located before the monochromator. Both of these shutters must be open to allow x-rays to enter the hutch. The hutch door interlock is tied to these safety shutters and beam cannot be present in the hutch while either of the door interlocks is open.

In addition to the safety shutters, there is a series of vacuum valves (two before and one after the monochromator) that also must be open before beam can be let into the hutch. All are controlled through the Interlock Control Panel, shown below in Figure 11. The vacuum valves should remain open through-out the user experiments, however if for some reason they are closed (red led), they can be opened in this order:

1. VALVULA SETOR 1;
2. VALVULA SETOR 2 and
3. VALVULA GATE ANEL.

To allow beam into the hutch, ensure all four keys are present and 'turned on' and press the 'ABRE/FECHA LINHA' switch. Note



Figure 11: Interlock Control Panel

the VAC SHUTTER is not relevant for user experiments and should remain open at all times.

To switch off the beam, simply press the 'OBTURADOR FEIXE BRANCO' switch. If no hutch doors are opened, the beam can be switched on again by pressing this same button.

There is a master control system that interfaces with the LNLS controls. This system controls and monitors vacuum and cooling lines for each beamline. For most users, this system will operate 'behind the scenes', but for certain problems, it is useful to be aware of this system-for example, if it is locked out by an administrator or detects an error in the system, it will not let the safety shutters open, and this must be resolved before experiments can continue.

If for any reason it is not possible to open the beamline to x-rays call the local contact or the control room at 1155/1156 for assistance.

6 Beamline Control Software

The beamline can be controlled from IMX1-LINUX computer on the beamline, running Red Hat. This computer is connected to the NI PXI and can control beamline components through EPICS or direct triggering, as outlined in Data Acquisition Architecture Section. It is also connected to the storage center, which allows interaction with the raw data and access to the reconstruction machine – mounted directly in the data center. A local user account is used for this computer (it should already be logged in and ready to operate if not, the login information is on a tag on one of the monitors). Control is achieved through CS-Studio software and can be accessed by clicking the Eclipse icon on the desktop or on the top control bar

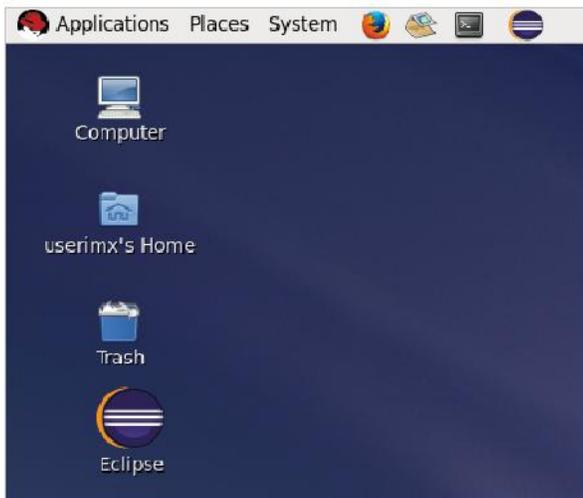


Figure 12: Start CS-Studio Control Software

Please note the coordinate system in use at the beamline:

- X: transverse to beam direction, positive towards hutch door;
- Y: Vertical direction, positive up and;
- Z: Beam direction, positive away from source.

6.1 CS-Studio

CS-Studio (Control System Studio), an open source toolset developed by Kay Kasemir of ORNL is the main graphical interface of the beamline. It comprises a set of Eclipse tools that can interact with EPICS PVs. Through CS-Studio, users can view all necessary beamline components, setup scan parameters, and monitor scan progress

through a single interface, as well as view the acquired images. For more elaborate routines, such as automated microscope focusing or sample and detector alignment, Python scripts handle and process raw data.

The default display brings up the Sample Window, shown below in Figure 13. Depending on the previous user, there maybe no sample image present. The software should normally be open and configured for the user, however, for completeness each of the control tabs will be detailed in this section.

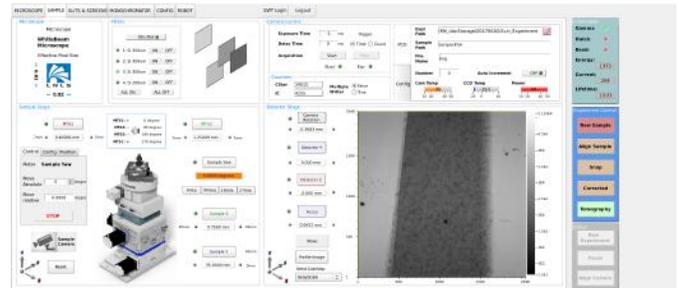


Figure 13: Default CS-Studio Screen

On the right hand side, the ring status is present along with information on hutch status, ring current, etc. Clicking on this window will display the history of the beam for the previous 12 hours - Figure ?? . Below this are a set of controls for running experiments and will be detailed below. On the top left hand corner are several tabs, to allow the user access all components of the beamline. Note, some of the controls maybe disabled for users if an administrator is not logged into CS-Studio.

6.2 Microscope Tab

In the Microscope Tab one of the staff member can change or focus the objective, adjust the detector to sample distance and change the detector height when switching between white beam and monochromatic beam. It is also possible to select which microscope is in use, through the CHANGE MICROSCOPE tab, and the objectives installed, using the CONFIG tab. However, **this should be setup by a member of staff before the experiment begins**. For the mono-microscope, it is possible to change the objective in use using the software. Simply click on ROTATE CW/CCW to change between Objectives 1, 2 and 3. For the white beam microscope, the objective can be retracted using the software, but needs to be

changed manually.

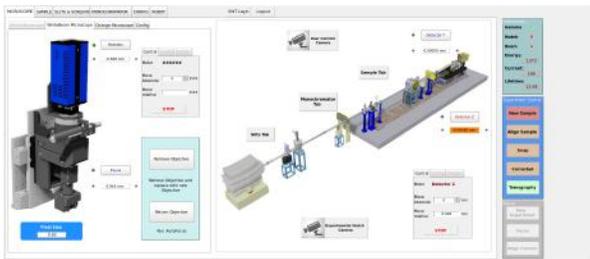


Figure 14: Microscope Tab

It is possible to adjust the detector position, click the button for the relevant stage: DETECTOR Y or DETECTOR Z. This stage will now be selected in the Control box, and the position can be adjusted by relative or absolute motion. Theoretically, for an image contrast based on x-ray absorption alone the detector should be placed as close as possible to the sample, on a practical sense, the detector distance should be smaller than the detector distance for phase contrast. The detector distance for phase contrast must respect the relation $z \ll \frac{d^2}{\lambda}$, d being the pixel size and λ the wavelength. Considering the magnification and pixels sizes available at the beamline you can use the table as guidelines:

- Monochromatic characteristics for PCO 2000 Camera (2048 x 2048 pixels, 7.4 μm x 7.4 μm):

Objective	Pixel Size (μm)	Detector Distance (mm)
2x	3.7	1000
4x	1.9	200
10x	0.74	25
20x	0.37	5

- White Beam characteristics for PCO 2000 Camera (2048 x 2048 pixels, 7.4 μm x 7.4 μm):

Objective	Pixel Size (μm)	Detector Distance (mm)
5x	1.64	100
10x	0.82	30

After such procedure it is necessary to align the camera rotation or focus the objective in respect to the scintillator, which can be done by calling the scripts embedded in the panel on the right hand side.

This procedure is done by a staff member and are described just for clarification on experiment procedures. Clicking on either the FOCUS or ALIGN CAMERA buttons will open separate windows, shown below in Figure ???. Here the range of motion through the stages will be scanned and can be determined along with the number of steps. While it is recommended to use the default values, it may be necessary to increase the range after changing the objective or moving the detector. It is important to remember to run both these functions when changing the sample-detector distance as the straightness of these stages is not perfect!

Note in all cases, always pay attention to the possibility of collisions between equipments, or samples. Keep in mind that whether moving a stage or running a scan, you can click the **STOP** button and stop all movement and cancel the scan.

Another point to note: clicking on any of the camera icons will open one of the three observation camera screens at the beamline; one for the sample, experimental hutch and beamline controls. This is in progress development, and so we do not recommend keeping those windows open. If used for too long, they will cause a buffer overflow and may cause the software to crash!

6.3 Sample Tab

This is your main window for beamline control and can be viewed in its component parts for positioning the sample, setting acquisition parameters and previewing images. The Sample Stage is used to position the sample in the FOV, as outlined in *Sample Aligning*.

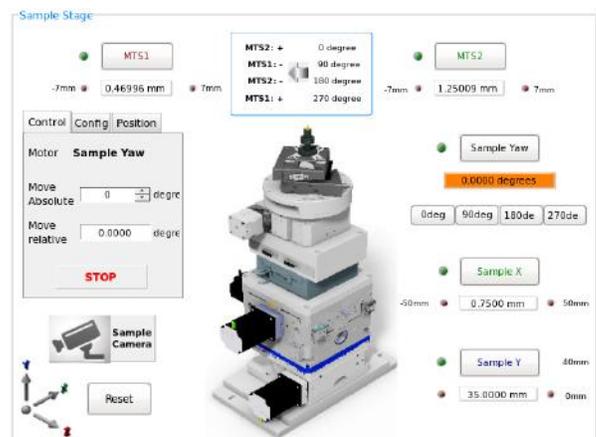


Figure 15: Sample Stage Positioning

Here it is possible to control the SAMPLE Y (Vertical), SAMPLE X (Transversal) and SAMPLE YAW (Rotation) along with the fine positioning stages mounted above the rotation axis, MTS1 and MTS2. These stages are connected by a slip-ring through the rotation stage to allow 'endless' rotation. Simply click on the stage to move, for example SAMPLE YAW above, and adjust the position, relatively or absolutely, in the control box. Note when the stage is selected, its name will display in the control box and its position indicator will change colour. Be sure to select the correct stage when moving!

Above the Sample Stage are some indicators showing the microscope in use and the effective pixel size in horizontal and vertical. The effective pixel size is based on the actual pixel size of the CCD, combined with the objective magnification and any software binning activated. There is also a section for Filters, which allows you to insert different thickness Si filters into the beam path before the sample. These filters can be used for fragile or heavy samples to cut-off the lower energies and can be used in any combination. It is recommended to use different filters combination to optimise the contrast on the measured image.



Figure 16: Microscope information and Filter control

In the Camera Control section all parameters relating to acquisition can be manually adjusted. Firstly, always ensure the experimental path is complete. The EXPT PATH is the storage location and should always include the storage location (either 'IMX_ddn_Storage' or 'Storage'), the user folder (based on proposal number eg. '20150001') or 'Storage'), the user folder (based on proposal number eg. '20150001') and experiment name (eg. 'Test_Experiment'). This file path is predetermined and should not change unless instructed by a IMX staff. Within this location, many samples can exist and this is shown in the SAMPLE PATH. Finally the image name and number can be changed to suit. This ensures the images are stored in the correct location and can be accessed by the user. To take an image, click START, and the preview will be updated. The two counters, CSTAR

(Cyberstar counter just before the sample) and IC (Ion Chamber before the fast shutter) will also update with beam intensity values.

The camera and triggering system has several modes of operation, which can be changed by clicking on the CONFIG tab within the Camera Control section - Figure 19. As shown below, it is also possible to change BINNING, ROI, and readout properties such as the number of ADCs and PIXEL CLOCK.

To change the trigger type, click on the TRIGGER drop-down panel and choose an option. EXP START is the simplest, where the exposure duration is controlled by the camera and the duration is set by the EXPOSURE TIME panel, in milliseconds. However, when changing the exposure time it is necessary to always click on UPDATE SETTINGS! With EXP CONTROL, the exposure duration is controlled by other devices, such as the NI PXI or the counters. In this case, it is not necessary to update settings and the duration can be controlled in the same manner by setting the EXPOSURE TIME. In this mode, it is also possible to control the exposure duration by the counters. This function is particularly useful for long scans where the decrease in beam current will cause a significant difference in image quality – typically more than 1 hour. To enable this mode, adjust the exposure time until a suitable image is obtained, note the CSTAR count value and then choose the control option COUNTERS and place this value (or similar) in the COUNT VALUE. Each image acquired will now have a variable duration, until this count value is reached and the exposure will stop

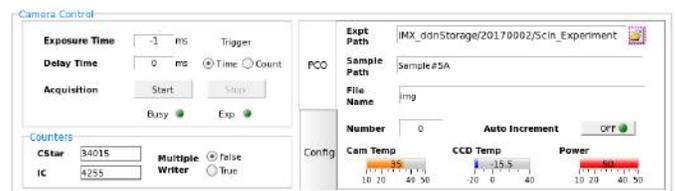


Figure 17: Camera Configuration

On the bottom of this screen is the DETECTOR STAGE panel, which shows the detector positions and the image preview. Placing the mouse over this image will show the pixel coordinates and the pixel intensity. Images are 16bit, thus saturate at 65535 pixel intensity counts. This information is useful when setting both the filters and the exposure before an experiment so get good contrast levels.

Clicking on the Profile image, another window will pop-up in which two lines can be positioned on the preview image to obtain a

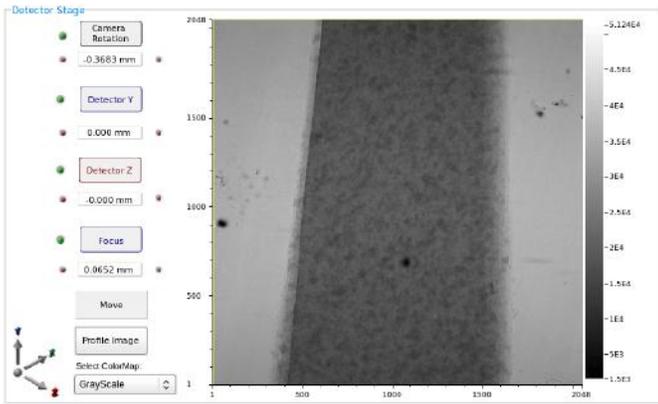


Figure 18: Detector Stage



Figure 19: Experimental Control

line profile. First drag those lines from the top edge or the left edge of the image.

6.3.1 Tomographic measurement procedure

Before discussing the remaining tabs and because this will be your main working tab during the experiment. It is important to point the procedure for creating a new sample folder, aligning and measuring a tomographic data set. To create a new sample, click on the NEW SAMPLE button in the Experiment Control panel. Here a pop up window will appear allowing you to set the sample name and add any description. After clicking the CREATE NEW SAMPLE, you will create a folder named after the sample where all the subsequent measurements will be save. Please note, no spaces can be used in any of the text fields. To close the windows click QUIT. For every new sample a new sample folder should be created to prevent accidental over-writing of experimental data.

6.4 Advanced setup

Before we start the description of this screen it is important to notice that the procedures described does not need to be frequently optimized, and so, we recommend asking for a beamline staff to optimize those parameters for your entire experiment.

6.4.1 Slits Tab

The Slits & Screens tab provides control for the pre- and post monochromator slits. The White Beam slits are on the left hand side, with the second set of high precision slits, before the sample,

on the right hand side. Both sets of slits consist of four blades which can be controlled individually. Again select the slit to move and enter the position in the Control box. There are some options to control the movements all slits, using just the horizontal or just the vertical, by using the HORIZONTAL SYNC, VERTICAL SYNC or SYNC ALL panels.

The slits can be manually adjusted to reduce the width of the beam to approximately the sample size. The main purpose for this is to reduce the total amount of light produced by the scintillator, thus minimizing artifacts from scattered light inside the camera box. When using monochromatic beam, the slits also cut the white beam from reaching the sample and being imaged.

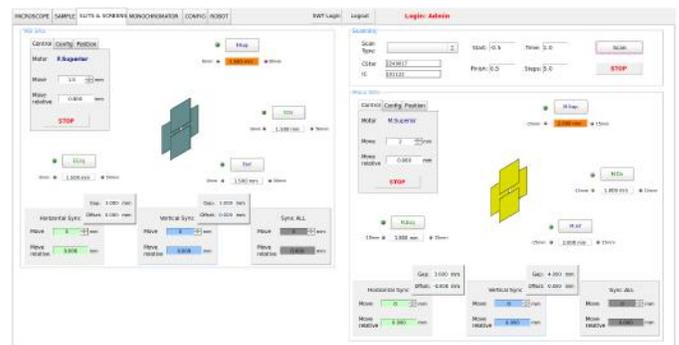


Figure 20: Slits & Screens Tab

On the bottom of this screen, is a temperature control for the thermal bath connected to the monochromator crystals. Mostly this is used as a display, however the temperature and flow rates can also be controlled from the software or directly on the bath itself. An

alarm system is incorporated into the software to alert the user if the bath level goes too low or if there are large temperature variations.

6.4.2 Monochromator Tab

The Monochromator Tab can be used to select between white beam and monochromatic modes. Clicking the drop-down box, highlighted in Figure 23 below, the local contact will select white beam or monochromatic beam using Si crystal or RuB4C multilayer. Once in place, it is possible to select the K-Edge to rotate the monochromator to the correct angle and adjust the monochromator height. The angle positions are provided in the appendix. The monochromator is not fixed exit, so the beam height downstream will be offset. This distance can vary from 6.6 mm to 13 mm depending on the crystal and angle used. Note, the height of the detector, post-monochromator slits and sample tower will have to be adjusted to account for this offset.

The temperature of the monochromator crystals and rotation motor are also monitored here and an integrated alarm system will notify the user if the temperature varies.

image in the specified path using name provided. Use the AUTO INCREMENT function to adjust the file number automatically so as not to overwrite previous data. It is useful to take a snap for every sample to easily see a preview of the sample for future reference.

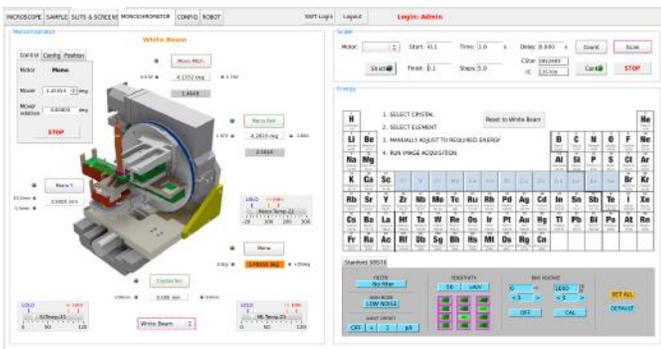


Figure 21: Monochromator Tab

The final Config tab is for configuring and controlling other motors, such as piezos, Talbot grating motors and fluorescence screens and is to be used only by beamline staff.

6.5 Experiment Control

Once the beamline is set-up, it is possible to start capturing useful data. Clicking START in the Camera Control panel takes an image, however, it is not saved. To save an image, click on SNAP in the Experiment Control panel. This will save a HDF and TIFF

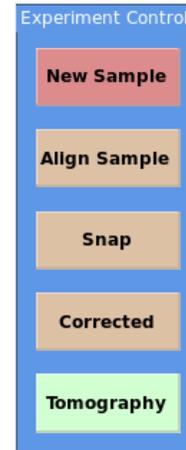


Figure 22: Experimental Control again

A corrected snap function is also available. This will first take a flat-field image, next a dark-field image, followed by the sample image and will save the corrected image. Click the CORRECTED button for this function. The first time called, the flat and dark images will be saved to the sample location. Subsequent corrected snaps will use the original flat and dark correction images.

The ALIGN SAMPLE function will take an image at 0 and 180 degrees, correlate both and attempt to position the rotation axis in the centre of the CCD sensor. For this function to work, the sample must be within the FOV at both these positions. It may take several iterations to reach the optimum position and is recommended to run for each sample also.

The TOMOGRAPHY button opens the tomography scan window, where the parameters for the particular scan can be input. This requires the start angle, finish angle and number of images. A typical scan consists of 1001 images over 180 degrees, but this will vary according to each user.

An option is available to change the tomography scan types and essentially how the instruments are triggered. EPICS SCAN simply sends all commands to take images, or move motor through EPICS and for scans with exposure times greater than 1 second is the best option. POINT-TO-POINT and FLY-SCAN both use

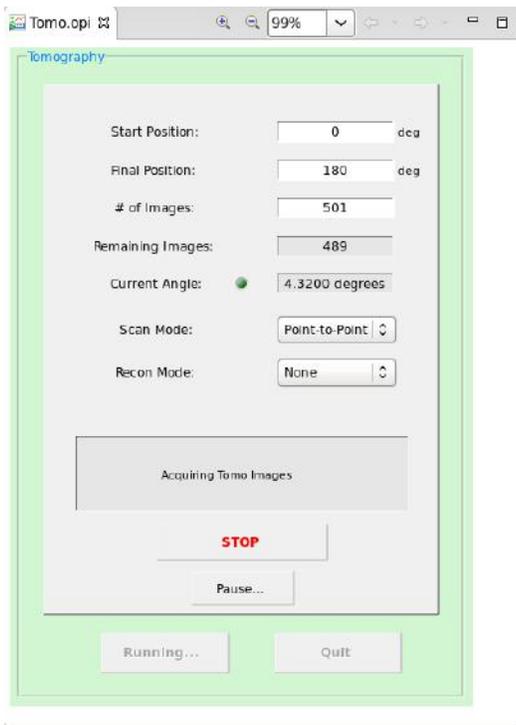


Figure 23: Tomography Scan

direct hardware triggering as opposed to sending variables through EPICS. This results in reducing the dead time by some 300ms per image and is a useful function for faster scan times. In POINT-TO-POINT scans the rotation stage stops at each point while the image is being acquired and can be used for scans from 100ms to many seconds. In FLY SCAN mode the rotation stage moves continuously, using an encoder to trigger the camera at the correct locations. These triggering systems are explained in more detail in the following section.

Another option allows for the acquired data to be reconstructed, as soon as the scan is complete. This particular option will be discussed in more detail in the Reconstruction Section below.

While the scans are complex in nature, there is minimal interaction with the user, requiring a few parameters at most to run a full experiment. CS-Studio interface calls all python/Py4Syn scripts to maintain consistency for the end user. The flowchart in Figure 25, shows the process flow in the usual tomography experiment performed at IMX. To perform fast scans, the execution separates into EPICS control and Hardware Control, which runs the scan independently from the motor record. In this occasion, the motor record

is used only for updating motor positions. Slow and non-sequential tasks stay controlled via EPICS while the sample rotation runs directly from DMC code. For frame rates higher than 5 Hz, the Uniblitz shutter control can be disabled to stay open during the entire acquisition. After the execution of the fast parcel, all PVs related to the motor record are updated.

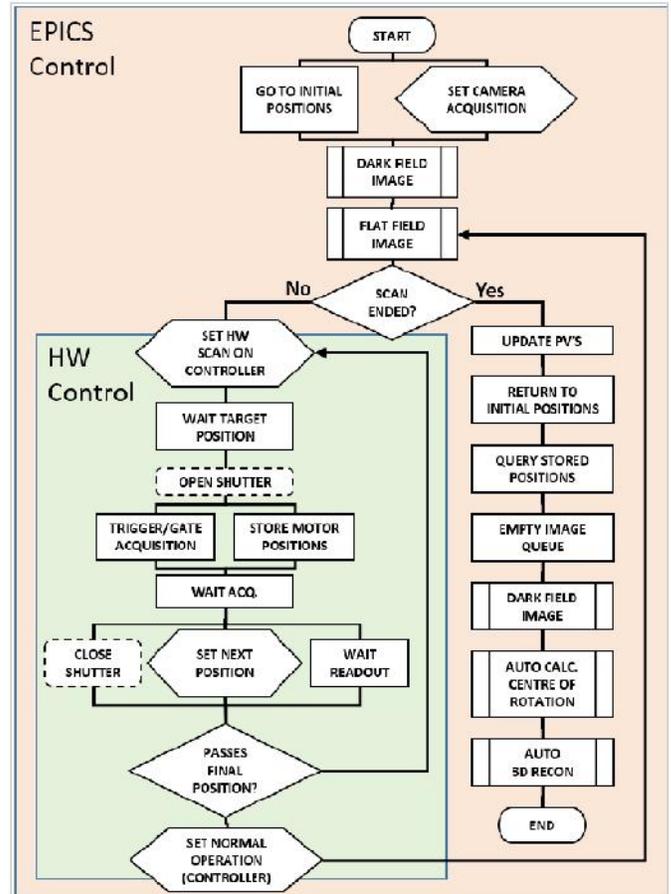


Figure 24: Experimental Flowchart

6.6 Triggering System

The experiment control system can be simplified to a three-layered architecture. The EPICS channel access protocol works as an intermediate layer (or “Service Layer”). It transfers information between low-level device drivers and the high-level user interface. The graphical user interfaces and experiment command sequences stay on the top layer, or so-called “Application Layer”, assigning parameters in the form of EPICS PV’s to EPICS IOC’s (Input-Output Controllers).

These IOC's on the "Service Layer" translate the parameters received from above into commands and signals to the device drivers on the layer below, the "Driver Layer". To connect the PXI's FPGA environment to EPICS Records, an in-house data exchange protocol called Hyppie creates a bridge between EPICS and the low-level hardware control. The FPGA side runs on LabVIEW Real-Time, as the EPICS side runs on Red Hat Linux. Arriving commands from the application layer land at the Linux side, passing to the RT side over shared memory on the PXI chassis.

Synchronisation can be achieved by sending commands through EPICS protocol, however, as already mentioned, this can result in significant dead time. To resolve this issue hardware synchronisation can be set through 5V TTL signals, exchanged between the scan participants, and centralized at the NI PXI-6602 board; resulting in faster scan times. Figure 26 shows the IMX beamline context diagram for experiment control.

various angles and extract the sinogram directly by changing the stack's cutting plane dimension. This data can then be accessed by other machines on the network to processes this data.

In the data route from the camera to the storage, the network configuration in test phase at IMX relies on big package transmission to minimize package loss and network latency. Package size and number of coalescence buffers are high, and all the network switches between the camera and the storage have QoS (Quality of Service) priority configuration. The storage is a GPFS file system with the purpose of providing better cost-effective scalability. With such configurations, the data transfer rate reaches 100 MB/s, or around 12 fps at full resolution. On the Camera Control application, a queue system is included to account for any additional latency on the network.

For faster acquisition rates, a 1GB internal storage is available on the camera. However, given the flux and intensity currently available at the LNLS storage ring, the use of binning is necessary for acquisitions with an exposure time of less than 50ms. As binning reduces file size, in some settings it is also possible to store an entire scan on the camera's internal memory, thus removing the readout time incurred during image transfer.

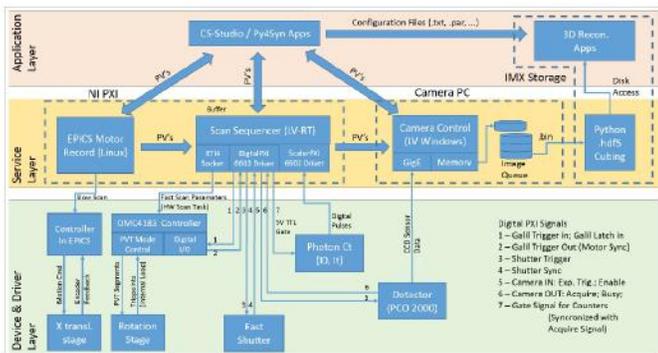


Figure 25: Data acquisition architecture using EPICS Records and LabVIEW drivers

6.7 Data Flow Path

A dedicated machine running Windows OS controls the PCO 2000 camera through a GigE interface. The machine has two network boards to handle high data throughput during scans. A dedicated TOE (TCP/IP Offload Engine) network board receives data directly from the camera, and a second network card sends data to the data storage location. Images are stored in RAW format and converted to an image format depending on the function called. The RAW data is subsequently removed. For the purpose of tomography reconstruction, all RAW data are stacked into a single HDF5 format image. In this way, it is possible to retrieve each projection for the

7 After the Experiment

7.1 User Space

As the beamline is continuously in use, it is important that the user removes all samples from the beamline, discards all consumable materials used for sample preparation and fixing and returns the beamline to the state at arrival.

7.2 Data collection and transfer

The LNLS provides users with a login account installed approximately one week before the experiment starts and removed automatically four weeks after the experiment ends. Data will be kept 30 days after the creation date. Both the account and the data will then be removed by automatic procedures, without prior notice.

So, users should save the data right after the experiment or transfer it in the following weeks.

8 Reconstruction Software

Depending on the option selected when running the tomography it is possible to begin a fully automated 3D reconstruction as soon as the scan ends, using in-house software Raft. While it is possible to reconstruct the full data set, it is recommended to reconstruct a single or a few slices initially. There are numerous parameters that can be adjusted depending on the sample, its size, the distance to the detector and the type of scan implemented.

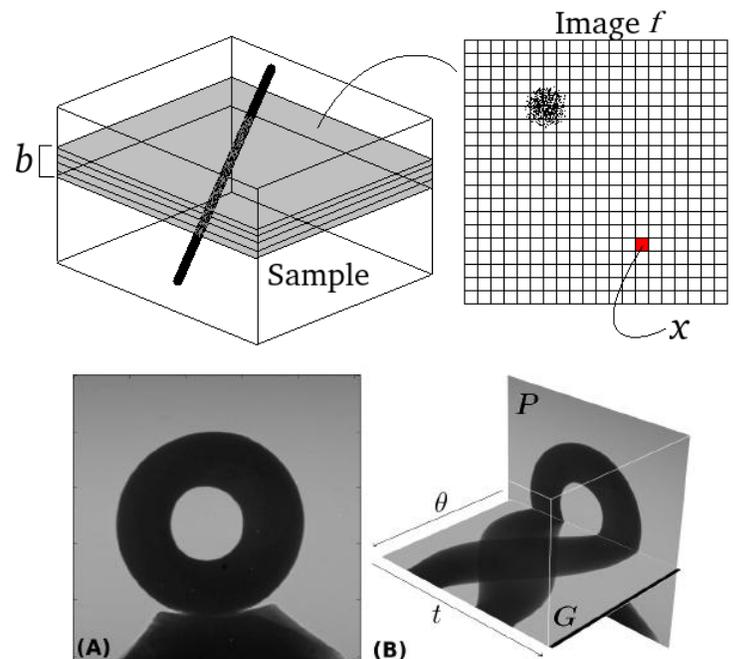


Figure 26: Left: 3D representation of an arbitrary sample. Right: image representation of a slice within a block of size b . Image P indicates a projection image while G is referred as a sinogram.

Theory: brief description

Most of the reconstruction softwares use the Radon transform and its inverse as the mathematical basis for reconstructing tomographic images. This function is often referred to as a sinogram because the Radon transform of an off-center point source is a sinusoid. The backprojection operation simply propagates the measured sinogram back into the image space along the projection paths. Inversion, or simply reconstruction, is done by analytical formulas or iterative methods. The classical mathematical approach is given by the classical filtered backprojection algorithm.

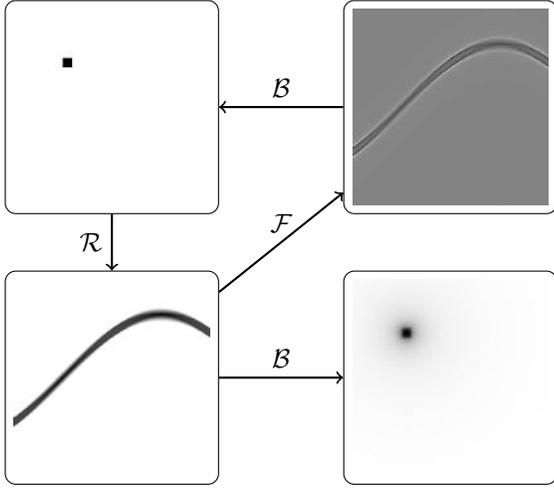


Figure 27: Radon \times Backprojection.

Figure 26 presents a stacking representation of the 3D reconstruction. Each slice within a block is represented by a two-dimensional function $f(x)$, being x a two dimensional *pixel* on the reconstructed image. A sequence of projections P is measured, each for an angle θ , determining an image G with coordinates (t, θ)

Inverse Problem: Can we restore the slice image f using the measured image G ?

The answer is yes! Each pixel x has an intensity $f(x)$ indicating the linear absorption coefficient. Image $G(t, \theta)$ is a discrete realization of the *Radon transform*, an integral operator defined as

$$G(t, \theta) = \int_{\mathbb{R}^2} f(x) \delta(t - x \cdot \xi_\theta) dx, \quad \xi_\theta = (\cos \theta, \theta)$$

We indicate \mathcal{R} as a symbol for the Radon transform, in the sense that $G = \mathcal{R}f$. If f is a point source function (a delta distribution), function G behave like a sinusoid in the (t, θ) space. This is the reason of why images G are called *sinograms*. The transposition of the Radon transform provide another integral operator, called *backprojection* and deescribed by the symbol \mathcal{B} . The backprojection operator \mathcal{B} operate over sinograms providing a blurred version of the original function f . It is a well known fact that $\mathcal{B}\mathcal{R}f$ is a convolution of f with the point-spread function $1/\|x\|$, providing a typical blurring effect. The action of \mathcal{B} over a sinogram is to determine an average of the measurements over all the straight lines passing through a pixel x . The definition of \mathcal{B} over the sinogram

H is

$$\mathcal{B}H(x) = \int_0^\pi H(x \cdot \xi_\theta, \theta) d\theta$$

Whenever H is a low-pass filtering of G over the axis t , $\mathcal{B}H$ determine the inverse f by means of the so-called *filtered backprojection* algorithm. A low-pass filter is computed through a convolution, typically computed using another integral operator called the Fourier transform.

Typical Artifacts

There are two important artifacts arising in image reconstruction from projections.

Ring artifacts: The first is a ring shaped artifact, arising from straight lines in the sinogram space. In fact, a transformation from polar (sinogram) to cartesian coordinates (feature image) always transform a straight line to a circle, as shown in Figure 28.

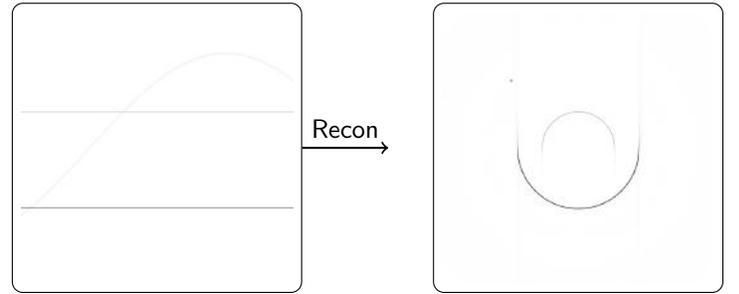


Figure 28: Ring artifacts on the feature image (right) obtained from a corrupted sinogram (left) using an inversion algorithm.

Solution: There are several algorithms for ring artifacts reduction. The one implemented for IMX can be found in the software description, at the end of this section. We denote \mathcal{S} as the filter operation, reducing or supressing stripes in the sinogram image, therefore reducing rings in the final reconstructed image. The sinogram is divided in N blocks of sinograms $\{G_1, G_2, \dots, G_N\}$, as shown in Figure 29; each block is then filtered C times with operation \mathcal{S} :

$$\tilde{G}_k = (\mathcal{S} \circ \dots \circ \mathcal{S})(G_k) = \mathcal{S}^C(G_k)$$

Here \mathcal{S}^C is a composition of operator \mathcal{S} . The filtered block \tilde{G}_k is now part of the new restored sinogram. Further details about the action of \mathcal{S} can be found in the manuscript (•).

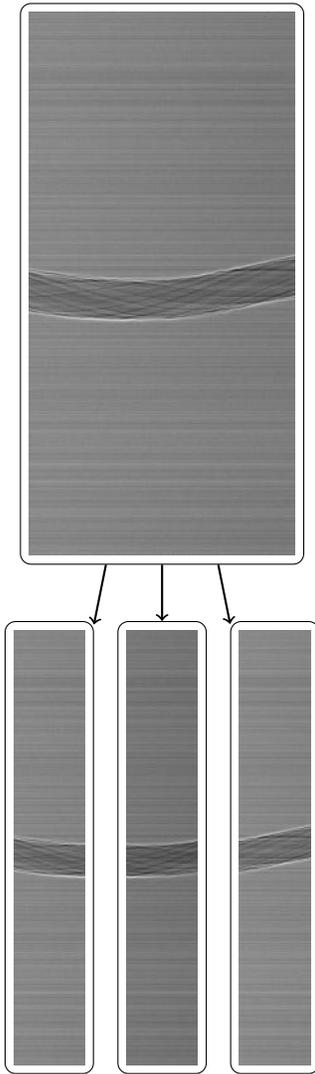


Figure 29: Sinogram division by blocks for ring suppression.

Arc artifacts: This artifact arise due to an offset of the center of rotation of the sample. If G is a theoretical sinogram, there are no jumps from angle $\theta = \pi$ to $\theta + \Delta\theta$. This can be seen concatenating the sinogram image G with his flipped counterpart (up down) image $F(G)$. As shown in Figure 30, the original sinogram G concatenated with his flip $F(G)$ has a strong jump at $\theta = \pi$, generating a strong arc artifact in the reconstructed image.

Solution: Users have to provide an average value for the offset, say $o \in \mathbb{Z}$, using the reconstruction graphical user interface available at the beamline. The reconstruction code will search for the best

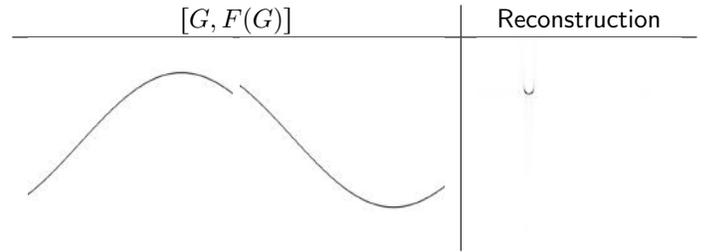


Figure 30: Reconstruction without center. Sinogram G and his flipped version $F(G)$ with a jump at $\theta = \pi$. The jump produce an arc artifact in the reconstructed image.

matching center of rotation β with subpixel precision satisfying

$$\|G(t - \beta, \theta) - F(G(t + \beta, 0))\|^2 < \epsilon$$

where F is the flipping operator and $\epsilon > 0$ a given precision. This an optimization strategy having $o \in \mathbb{Z}$ as a starting point. It is important to note that *users are responsible to search the best starting point o . Misleading numbers will provide reconstruction with arc artifacts. The graphical interface provide an easy way to search the best matching point o .*

Edge Enhancement

Samples with low absorption can have a significant increase of contrast using a regularization parameter α . This is a consequence of a Tikhnov regularization in the least squares sense, providing a generalized filtered backprojection approach. The details can be found in the associated manuscripts to the software description.

An example using tomographic projections from a kapton tape is shown in Figure 31. The value of α improve contrast for an almost non absorbing sample. This strategy is similar, but not identical to the one proposed by Paganing *et al*. This strategy can be described as a filter approach on the sinogram G using the following convolution operator

$$\tilde{G}(t, \theta) = G(t, \theta) \star M(t), \quad \hat{M}(q) = \frac{|q|}{1 + 4\pi^2\alpha q^2}$$

with $\hat{\cdot}$ indicating the Fourier transform of M .

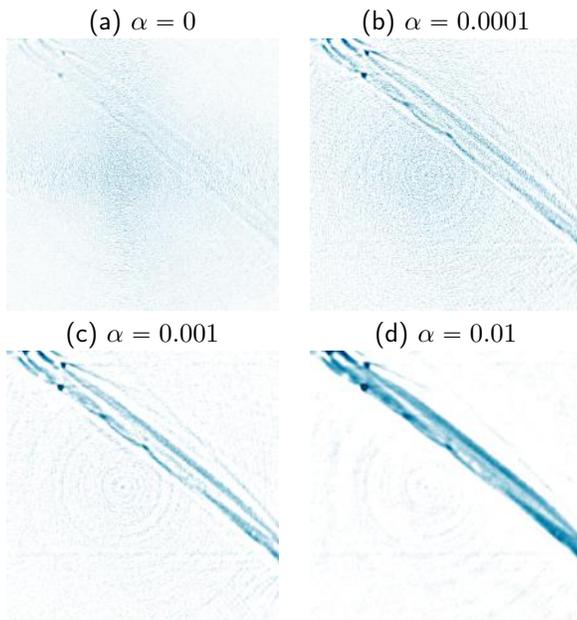


Figure 31: Effect of regularization parameter.

Software Description

The software is able to run on computers equipped with a GPU and at least 8Gb of RAM. In-house development automatically calculates sample's center of rotation and other reconstruction parameters are set according to the beamline conditions. However, it may be necessary to adjust the intensity of ring filters, CCD filters, or activate the Paganin function for phase contrast reconstruction.

Download

Codes are not freely available for download. Interested users should request them sending an email to eduardo.miqueles@lnls.br. As soon as we reach a stable version, the code will be hosted on a public git-hub account:

<https://github.com/exmiqueles/raft>

Dependencies

- Cmake <https://cmake.org/>
- HDF5: <https://support.hdfgroup.org/HDF5/>
- CUDA-8.0: <https://developer.nvidia.com/cuda-toolkit>
- FFTW3: <http://www.fftw.org/>
- Boost: <http://www.boost.org/>
- Blas: <http://www.netlib.org/blas/>

- Lapack: <http://www.netlib.org/lapack/>
- Libnfft: <https://www-user.tu-chemnitz.de/~potts/nfft/>
- Gengetopt: <https://www.gnu.org/software/gengetopt/gengetopt.html>
- Python: Numpy/scipy/scikit-image/Matplotlib/h5py

Minimal Working Example

Run the bashscript `install` to compile the source code and add execution files within the folder `bin/`. Users will have to include `bin/` in their environmental variable `$PATH` to run `raft` scripts locally.

We assume that all *.h5 files are located in the tomographic folder `tomo/folder/` with the following structure:

```
tomo/folder/
|-- recon/
|-- tomo_dark_before.h5
|-- tomo_flat_after.h5
|-- tomo_flat_before.h5
|-- tomo\_flats.h5
|-- tomo.h5
```

To reconstruct a single folder, run the following line command

```
/bin/raft -p /tomo/folder/ -i 334 -f 667 -b 16 -o 2
-c 2 -d 3
```

All reconstructed slices will be placed in `/tomo/folder/recon/` as a sequence of binary files. The above line command reconstruct 333 slices between initial slice 334 and final 667 using a block of 16 slices to communicate with the GPU (see flag `b` in Fig.26); with initial shift of 2 pixels, ring composition 2 and rings-division set to 3. Type `raft -help` for a complete list of reconstruction options.

Publications

- Miqueles, Eduardo X., et al. "Generalized Tikhonov's algorithm for ring artefacts reduction." *Journal of synchrotron radiation* 21.6 (2014): 1333-1346.
- Miqueles, Eduardo X., et al. "Fast Backprojection Techniques for High Resolution Tomography", <https://arxiv.org/abs/1608.03589>, 2016.
- Miqueles, Eduardo X., et al. "Phase Retrieval as Regularization Problem", <https://arxiv.org/abs/1702.05092>, 2016.

A publication of the software is under development. More sophisticated algorithms are being implemented, especially iterative reconstruction, using high-performance computing and will be detailed as they become available.

A K-Edge angles for multilayer and Si crystals.

ATOMIC NAME	ATOMIC SYMBOL	ATOMIC NUMBER	K ABSORPTION EDGE [Å]	K ABSORPTION EDGE [KEV]	WAVELENGTH [µm]	ML ANGLE	SI ANGLE (2dSinθ)
Magnesium	MG	12	9.51220	1.3033	0.000951431	-	-
Aluminium	AL	13	7.94813	1.5598	0.000794974	-	-
Silicon	SI	14	6.73800	1.8400	0.000673913	-	-
Phosphorus	P	15	5.78400	2.1434	0.000578520	-	-
Sulfur	S	16	5.01850	2.4704	0.000501943	-	-
Chlorine	CL	17	4.39710	2.8195	0.000439794	-	-
Argon	AR	18	3.87090	3.2028	0.000387161	3.770520800	38.126522559
Potassium	K	19	3.43650	3.6076	0.000343719	3.355729500	33.238346728
Calcium	CA	20	3.07030	4.0379	0.000307090	3.000985800	29.321668747
Scandium	SC	21	2.76200	4.4886	0.000276255	2.700969300	26.138356704
Titanium	TI	22	2.49734	4.9643	0.000249783	2.442756900	23.473560642
Vanadium	V	23	2.26910	5.4637	0.000226952	2.219828400	21.218006992
Chromium	CR	24	2.07020	5.9886	0.000207060	2.025319200	19.280644241
Manganese	MN	25	1.89643	6.5374	0.000189678	1.855221900	17.606400285
Iron	FE	26	1.74346	7.1109	0.000174380	1.705555000	16.145729715
Cobalt	CO	27	1.60815	7.7093	0.000160845	1.573074700	14.862281972
Nickel	NI	28	1.48807	8.3314	0.000148835	1.455551400	13.729842388
Copper	CU	29	1.38059	8.9800	0.000138085	1.350352300	12.720865225
Zinc	ZN	30	1.28340	9.6600	0.000128364	1.255212500	11.811980290
Gallium	GA	31	1.19580	10.3677	0.000119602	1.169364600	10.995262970
Germanium	GE	32	1.11658	11.1032	0.000111680	1.091832600	10.258737759
Arsenic	AS	33	1.04500	11.8638	0.000104520	1.021725800	9.594602083
Selenium	SE	34	0.97974	12.6540	0.000097993	0.957874550	8.990314722
Bromine	BR	35	0.92040	13.4698	0.000092058	0.899789500	8.441709266
Krypton	KR	36	0.86552	14.3239	0.000086569	0.846084650	7.935002017
Rubidium	RB	37	0.81554	15.2018	0.000081569	0.797168830	7.474058814