ANATOMIX Beamline User Guide

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ANATOMIX Beamline User Guide

Author:

Timm Weitkamp
Synchrotron SOLEIL
L'Orme des Merisiers
Départementale 128
91190 Saint-Aubin
France
weitkamp@synchrotron-soleil.fr

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Chapter 1

About this document

1.1 Purpose of this document

The ANATOMIX Beamline User Guide is there to give users of ANATOMIX beamline-specific information to help them use the beamline.

The information in the ANATOMIX Beamline User Guide is ultimately meant to cover all stages that users need to go through, from first contact with the beamline staff via the preparation of their beamtime proposal, preparation of the beamtime till after the experiment has ended, including the publication phase.

It is an evolving document. We are trying to get ahead with including more and more relevant information, but it will probably never be complete.

1.2 What this document is not

A general SOLEIL user guide. The ANATOMIX Beamline User Guide is not meant to give information common to all beamlines at Synchrotron SOLEIL. In particular, you will not find information in this document that explains the general procedures for applying for beamtime, declaring participants and samples, submitting end-of-run reports and experiment reports, making travel bookings, or other administrative aspects of beamtime preparation. For this information, we kindly ask you to refer to the SOLEIL web site, www.synchrotron-soleil.fr.

A primer on synchrotron tomography. It is also not within the scope of this document to give an introduction into the principles of microtomography or X-ray microscopy. Suitable textbooks and review articles on these subjects include Kak and Slaney (1987), Als-Nielsen and McMorrow (2011) on basic principles, and Stock (2008a), Banhart (2008), Stock (2008b), Maire and Withers (2014) on aspects more focused on application.

A citable reference on the beamline. As a reference with a description of the beamline, please do not cite this guide, but rather an article published in a scientific journal (⟶ page 39, "Cite beamline reference paper").

1.3 Where to get the latest version of this document

You can download the latest version of this document from the ANATOMIX web pages at https://www.synchrotron-soleil.fr/en/beamlines/anatomix. That page also contains more information on the ANATOMIX beamline.

1.4 Disclaimer

Although we are constantly working to keep the information in this document as correct, exact and up to date as possible, parts of this document may at times be outdated. When in doubt about any detail, ask the beamline staff.

Chapter 2

Introduction

2.1 About ANATOMIX

ANATOMIX is a beamline for X-ray tomography on the micro- and nanoscale, in absorption and phase contrast. It operates in the energy range from 5 keV upward and allows its users to obtain two- and three-dimensional radiographic images of bulk volume samples of macroscopic size (up to several cm thickness). For smaller samples, a spatial resolution down to 100 nm (30 nm pixel size) is available. Real-time studies are possible at speeds of up to one microtomography scan per second, and tests have been performed in which up to 20 microtomography scans per second were successfully acquired.

A sample interface designed to be as flexible as possible is meant to enable *in situ* and/or *operando* studies under conditions similar to the natural or working environment of the samples (temperature, humidity, mechanical load, transport processes). Biological samples can usually be measured without dehydration and, in many cases, without chemical fixation.

2.2 Experimental techniques on ANATOMIX

Two classes of radiographic methods for two-dimensional (2D) or three-dimensional (3D) X-ray imaging are available: first, **parallel-beam microimaging** (also referred to at the beamline as **microtomography** or **microradiography**); second, **transmission X-ray microscopy** (TXM), which we also refer to as **nanotomography** when it is used in tomography mode. Table 2.1 lists some important characteristics and differences of these two types of methods.

2.3 Basic principles of tomography at ANATOMIX

This section presents a few principles of tomography at the ANATOMIX beamline which are useful to know in comparison with other synchrotron tomography stations, or with laboratory setups.

Table 2.1: Main two techniques offered at the ANATOMIX beamline.

	Parallel-beam microimaging ("microtomography")	**Transmission X-ray microscopy** ("TXM nanotomography")
Principle	"Simple" projection radiography	Magnified imaging via X-ray lenses
Photon energies	from 10 to 50 keV ($\lesssim 25$ keV with monochromatic beam)	5 to 11 keV, 17 keV (always monochromatic)
Resolution	down to ≈ 0.5 µm	down to ≈ 80 nm
Typical pixel size values	0.325 µm, 0.65 µm, 0.87 µm, 1.3 µm, 3.1 µm, 6.5 µm, 13 µm	20 to 80 nm
Field of view	typically 2000× pixel size, within the limits of beam size (max. 40 mm width, 15 mm height)	$\approx (40 \text{ µm})^2$ (limited by illumination)
Contrast modes	Absorption contrast, inline phase contrast	Absorption contrast, Zernike phase contrast
Local scans	Possible	Possible
Offset scans	Possible	Possible

2.3.1　Always parallel beam, always filtered backprojection

Regardless of the details of your experiment, or even of the experimental station you are using (microtomograph or TXM), all tomography data acquired at ANATOMIX can be considered as fulfilling the parallel-beam approximation, i.e., the raw projection images are considered to be projections along parallel rays that are all perpendicular to the rotation axis. This means that each axial slice of the resulting volume can be computed independently of the neighboring slices.

The reconstruction software used in the standard data processing pipeline at ANATOMIX is PyHST2 (Mirone et al., 2014), developed at the European Synchrotron Radiation Facility (ESRF) in Grenoble. It uses the well-known algorithm known as *filtered backprojection* to compute the slices of the reconstructed volume. An option included in PyHST2 and frequently used at ANATOMIX for the reconstruction of inline phase-contrast microtomography data is the "Paganin filter" for semi-quantitative phase retrieval (Paganin et al., 2002; Weitkamp et al., 2011).

2.3.2　All scans on the fly

All tomography acquisitions on ANATOMIX are performed *on the fly,* i.e., the rotation axis does not stop turning while the projection images are acquired. This has several advantages over step-by-step scanning (in which the rotation is interrupted at each projection angle), including

- shorter scan times (no dead times induced by start–stop sequences),

- better data quality for local tomography (out-of-field contributions are blurred, reducing structured noise in the reconstructed volume).
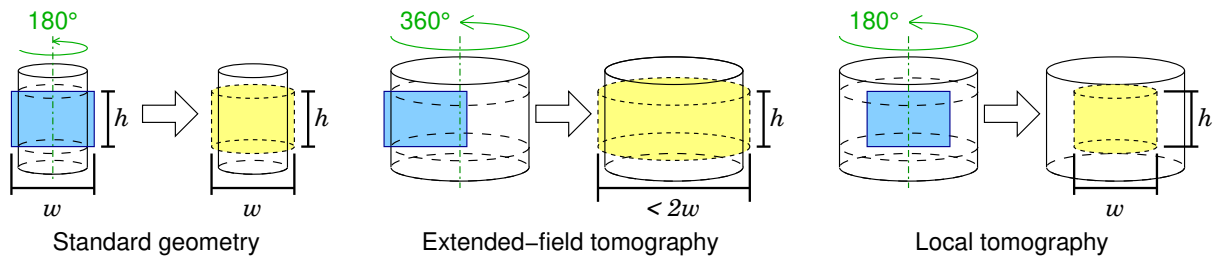
Figure 2.1: Tomography geometries. White cylinders represent the sample. Blue rectangles indicate field of view of the detector (width w, height h). Yellow cylinders indicate the reconstructed volume. Green dash-dotted lines indicate the axis of rotation. Angle values (in green ink) indicate the required angular range of the tomography scan.

The exact implementation of the on-the-fly scanning procedure (synchronized, non-synchronized, data storage location etc.) may vary; for more details on these aspects, see section 5.2.

2.3.3   Local and extended-field tomography possible

In the "standard" geometry for parallel-beam tomography (left panel in Figure 2.1), i.e., both for microtomography and for nanotomography on ANATOMIX, the sample stays inside the horizontal field of view during the scan. The reconstructed volume will be a cylinder whose diameter and height will equal, respectively, the width w and height h of the detector field of view. Since the beam can be considered parallel, projections taken at angles 180 degrees apart from one another are equivalent, so that an angular range of 180 degrees for a full tomography scan is sufficient. In general, the diameter of the reconstructed volume region is limited to the width of the detector field of view (or the width of the beam, if the beam is smaller than the detector).

If the horizontal dimensions of the sample exceed the field of view, there are two mutually non-exclusive ways of dealing with this problem: extended-field tomography and local tomography.

Extended-field tomography (sometimes also called "half acquisition" or "offset scan"; Figure 2.1, center): the sample stage (rotation stage and sample itself) is positioned with a lateral displacement relative to the X-ray beam and detector, so that the rotation axis is located near the edge of the field of view. The tomography scan is then performed over a range of 360 degrees, rather than the 180 degrees that are sufficient in standard geometry. In this way, by stitching together projection images taken at view pairs separated by 180 degrees, the reconstructed volume can be extended in the two dimensions perpendicular to the rotation axis by almost a factor of two. In other words, the diameter of the reconstructed volume will now be extended to slightly less than $2w$ (twice the detector field of view), while its height remains the same as for a standard scan in standard geometry. Since, compared to a standard scan, the angular sampling density needs to be doubled, in addition to the requirement of twice the angular scan range, an extended-field scan will require 4× as many projection images and produce 4× more raw data than a standard-geometry scan taken with the same detector configuration. The computing time for reconstruction will be substantially longer, and the reconstructed volume is also four times larger.

Local tomography (also called *region-of-interest [ROI] tomography*, Figure 2.1, right) simply means that the dimensions of the sample perpendicular to the rotation axis exceed the field of view, i.e., the sample diameter is larger than the horizontal field of view. This will have several implications that may affect the quality of the results:

1. Thicker sample usually means you will need to use a higher photon energy, which in turn typically results in weaker contrast of the features you would like to discriminate; it may also affect spatial resolution, scan time and other performance parameters.

2. Features in the object that are in the peripheral area outside the reconstructed volume will show up in some of the projection radiographs and create artifacts in the reconstructed volume data, typically in the form of salt-and-pepper noise. (This phenomenon is alleviated, but not totally eliminated, by the fact that the samples rotate continuously during the acquisition.)

3. The fact that the projection information is not complete ("truncated-projection problem", also known in mathematics as the "local tomography problem") makes it impossible to obtain quantitatively correct reconstructed values of the object function and in the most general case will result in cupping artifacts, i.e., regions of uniform composition in the sample will not be reconstructed with a uniform gray value, but their reconstructed values will depend on the distance from the rotation axis. The lack of quantitative correctness of the reconstructed values of object function is usually not a problem in studies that only need morphological information, not densitometric data. Cupping artifacts from truncated projections may make the segmentation of the data more challenging. This problem is aggravated for large samples with high eccentricity, i.e., in which the region of interest imaged is close to the periphery of the sample.

If the sample diameter is even larger than twice the field of view, extended field and local tomography can also be combined.

Both local tomography and extended-field tomography are possible on ANATOMIX in both the microtomography and the nanotomography (TXM) modality.

2.3.4   All reconstruction while you are at SOLEIL

The paradigm of data processing at ANATOMIX, like at many other synchrotron tomography beamlines, is that the tomographic reconstruction of all the data acquired is performed at SOLEIL, on SOLEIL computers, by the users while they are at the beamline, during the experiment and, where necessary, immediately afterwards. Moreover, the reconstruction software PyHST2 used at ANATOMIX, although distributed under an open-source license by its developing organization, the ESRF, is not easy to install.

2.3.5   Data file formats

The data produced in a tomography scan on ANATOMIX, including the data processing pipeline, are stored in various file formats. The file format that is of the greatest

importance from a user's point of view is raw binary floating-point format (`.vol`), because the reconstructed volume data are stored in this format. Other formats include Nexus (`.nxs`, a variety of HDF5) for the raw data, i.e., projection radiographs, "flat" and dark reference images, and single-frame ESRF Data Format (`.edf`) (Boesecke, 2013) for some auxiliary data created in the pre-processing steps after acquisition and prior to the actual tomographic reconstruction. Finally, some metadata and/or correction tables are stored in text format (various file name extensions including `.txt` and `.info`). The reconstruction parameters and selected metadata such as motor positions are also stored in a human-readable Ascii parameter file with the extension `.par`.

Reconstructed volumes   The tomographic reconstructions (volume images generated by PyHST2) are raw, 32-bit (i.e., single precision) floating-point data in little-endian byte order. Their filename extension is `.vol`. These files are not compressed, contain no header and no metadata whatsoever. However, for each `.vol` file, PyHST2 additionally generates a small, human-readable text file that has the same filename prefix as the volume-data file, but with the extension `.vol.info`. This small text file contains the dimensions of the volume data file and some additional information. (Equivalent information is contained in an XML metadata file also generated by PyHST2.)

Since the full reconstructed volume of each scan is stored in a single file, the `.vol` volume files are often very big. For example, a `.vol` file containing a $2000 \times 2000 \times 2000$-voxel volume will have a size of 32 GB.

Despite their usually impressive size, these files can be opened quite easily with common image display and processing software such as ImageJ (Schneider et al., 2012). ImageJ can also be used to export the images into a stack of single-image files, for example in TIFF format.

ImageJ is installed on the computers at the beamline and serves as the principal application to inspect data quality. To open a `.vol` file in ImageJ, select "File" $\longrightarrow$ "Import..." $\longrightarrow$ "Raw..." In the dialog box that will then open up, choose the following parameters:

Image type:	32-bit real
Width:	⟨x dimension in pixels; parameter `NUM_X` in .info file⟩
Height:	⟨y dimension in pixels; parameter `NUM_Y` in .info file⟩
Offset to first image:	0 bytes
Number of images:	⟨z dimension in pixels; parameter `NUM_Z` in .info file⟩
Gap between images:	0 bytes
White is zero:	no
Little-endian byte order:	yes
Open all files in folder:	no
Use virtual stack:	yes (if limited in memory)
	no (otherwise)

Projection images   The file format in which the raw detector data are first saved may vary according to the configuration of acquisition, but in the overwhelming majority of cases —those in which the Flyscan architecture is used— it is Nexus format. In this case, the raw data consist of one big Nexus file containing all the projection radiographs

and three much smaller Nexus files containing, respectively, the flat-field images recorded before the projections, the flat-field images recorded after the projections, and the dark images.

Legacy remark: The data processing chain used until spring 2022 implied a step in which the projections were converted to single-frame ESRF Data format (`.edf`). Since each of these `.edf` files contained only one detector frame, there were usually a few thousand of these files per tomography scan, and each file was relatively small, typically a few megabytes. Each of these files consists of an Ascii (text) header followed by the data as uncompressed, raw 16-bit unsigned integers. The header contains the information on image dimensions, data type etc. For each tomography scan, these images were stored in a subdirectory of the folder that holds the reconstructed volumes.

Chapter 3

Preparing an application for beamtime

3.1 Contacting the beamline scientists

The ANATOMIX beamline scientists are always happy to receive requests for information regarding potential projects you may have. Our contact details are listed in Table 3.1. They can also be found on the ANATOMIX beamline web page.

It is mandatory that you contact beamline staff before preparing a beamtime application.

3.2 Writing a proposal

Once you have exchanged with the beamline staff on your project, you can prepare a beamtime application proposal.

To apply for beamtime on ANATOMIX, typically via proposal submission in the semi-annual calls (deadlines mid-February and mid-September) the same rules as for all other SOLEIL beamlines apply; see the page *How to prepare a proposal?* on the SOLEIL web site. Proposals must be submitted via SOLEIL's *SUNset* web portal and contain a "general" part (a web form) and a two-page document *Abstract and experimental description* that can be prepared with a standard word processor, using a template accessible on *SUNset*, and needs to be submitted in PDF format.

As in all research projects, please do not include SOLEIL staff in the list of co-proposers unless you have their explicit and specific personal agreement.

Table 3.1: Names and contact details of the ANATOMIX beamline scientists.

Name	E-mail address	Telephone number
Jonathan Perrin	jonathan.perrin@synchrotron-soleil.fr	+33 (0)1 69 35 94 99
Mario Scheel	mario.scheel@synchrotron-soleil.fr	+33 (0)1 69 35 96 31
Timm Weitkamp	weitkamp@synchrotron-soleil.fr	+33 (0)1 69 35 81 37

In the "general part" of the proposal (the web form) there are a few questions that are not totally adapted to the full-field imaging techniques used on ANATOMIX, and can thus cause uncertainty as on how to fill them in and what information to provide. Others may ask for parameters that you are not sure about at the time of writing. Specifically:

- "Machine operation mode" can be left free, or you can choose "multibunch mode".

- "Photon energy range requested" should be filled in, but the 2-page free-text "Experimental description" (see below) should give more detailed information on sample size and composition, and other relevant elements that help the beamline scientists decide which photon energy, or range of photon energies, is best suited for the project.

- "Beam type": will be "white beam" for most, but not all microtomography experiments (if in doubt, leave it free) and "monochromatic beam" for all TXM experiments.

- "Spot size requested": here we advise you to enter the useful beam size illuminating the beam. In the case of a microtomography experiment, this will usually be the detector field of view; in the case of a nanotomography (TXM) experiment, it will be the field of view of the X-ray microscope (for example, 40 µm × 40 µm).

You will also be asked to declare your samples. Please note that any ancillary equipment you intend to bring to the experiment (e.g., power tools or other powered equipment, gas bottles, special sample environments such as furnaces, traction rigs, pressure cells, etc.), as well as any chemical products you may want to bring (solvents etc.), must be declared in this section too.

In the part *Abstract and experimental description* (a two-page document to be prepared with a standard word processor, using a template accessible on the *SUNset* platform) it will be helpful if you include in the section *Experimental method* all the information that we need to judge the technical feasibility and the basic parameters of the experiment. This information includes

- the size, shape and approximate composition and density of the samples;

- details on sample mounts that will be used during the measurements, especially if the samples are not free-standing (containers, for example);

- the size of the regions of interest to be imaged;

- the X-ray photon energy you plan to use (if known);

- the spatial resolution you intend to obtain or pixel size you intend to use, or the size and shape of details you intend to characterize from the measurements;

- whether the measurements will be static (samples remain unchanged during the measurement) or dynamic (samples undergo treatment or modification during the experiment, i.e., an *in-situ* experiment; in the latter case, provide details on the sample environment including actuators, sensors, heating or fluid devices etc. that you intend to install;

- the number of samples;

- any other relevant information.

If you send us your proposal draft by e-mail sufficiently ahead of the submission deadline, we will be try to give you feedback and advice. For obvious reasons, this becomes more and more difficult for us as the deadline approaches. Moreover, the proposal submission deadline is usually close to or within the school holiday period, during which some or all beamline staff members may be absent. We therefore advise you to send us your proposal drafts at least two weeks before the final submission deadline.

Chapter 4

Preparing your beamtime

This chapter describes the steps after your proposal has been accepted and before the actual experiment.

4.1 Number of experimentalists

A tomography beamtime usually requires more workforce than most other synchrotron beamtimes. This is mostly because

- the time for a single measurement, i.e., a tomography scan, is relatively short — typically on the order of a few minutes—, so samples must be changed (and aligned) in short intervals, and new samples must be prepared;

- the data processing during the experiment, usually just after the acquisition of each scan, requires interactive work and therefore keeps an additional person busy.

For simple and short experiments lasting only one or two days, it will be sufficient if two experimentalists from the user group are present. However, for more complex measurements and/or longer beamtimes, to ensure optimum shiftwork use of the instrument around the clock, we recommend that user groups should comprise around 6 people present on the SOLEIL site for the whole time of the experiment, so that there are at least two, better three persons attending the instrument all the time.

The best is to set up a roster already in the scheduling phase in the experiment, in agreement with all prospective experimentalists. If you are the one in charge of the experiment, this will give you a precise idea of how many people will be available at any given time. Figure 4.1 shows an example that a user of a particularly well-prepared experiment sent us before her beamtime.

If you cannot organize so many participants, it is of course possible to work with a smaller group (except for experiments classified "red" by the SOLEIL Safety Group; these require permanent attendance anyway), but this may affect efficiency.

|	Mardi 20 nov 06h-14h	Mardi 20 nov 14h-22h	**Mardi 20 nov 22h-6h**	Mercredi 21 nov 06h-14h	Mercredi 21 nov 14h-22h	**Mercredi 21 nov 22h-6h**	Jeudi 22 nov 06h-14h	Jeudi 22 nov 14h-22h	**Jeudi 22 nov 22h-6h**	Total créneaux
			1		1	1			1	4
		1	1					1	1	4
		1	1							2
				1	1		1	1		4
	1				1		1	1		4
	1	1		1		1	1		1	6
	1				1	1				3
			1	1						2
	1			1			1			3
									1	1
		1								1
Total personnes	4	4	4	4	4	3	4	3	4	

Figure 4.1: Example schedule prepared by the main proposer of an experiment on ANATOMIX, made a few weeks before the beamtime. (Experimentalists' names blurred for anonymity.)

4.2 Sample preparation and mounting

4.2.1 Free-standing samples

The standard way of mounting solid and rigid samples for measurements in air without specific sample environments is on Huber 1005 goniometer heads or compatible equipment (Huber Diffraktionstechnik, Rimsting, Germany, xhuber.de; see also Figure 4.3, left). Figure 4.2 shows a view of the microtomography station in the first experimental hutch of ANATOMIX with three detectors and a sample mount of this type.

The sample carrier pins designed to go into the goniometer head are generally not supplied by the beamline (although a small stock is available). If you want to use pins of this type, we advise you to buy a stock. Specifications and references are listed in Table 4.1; a
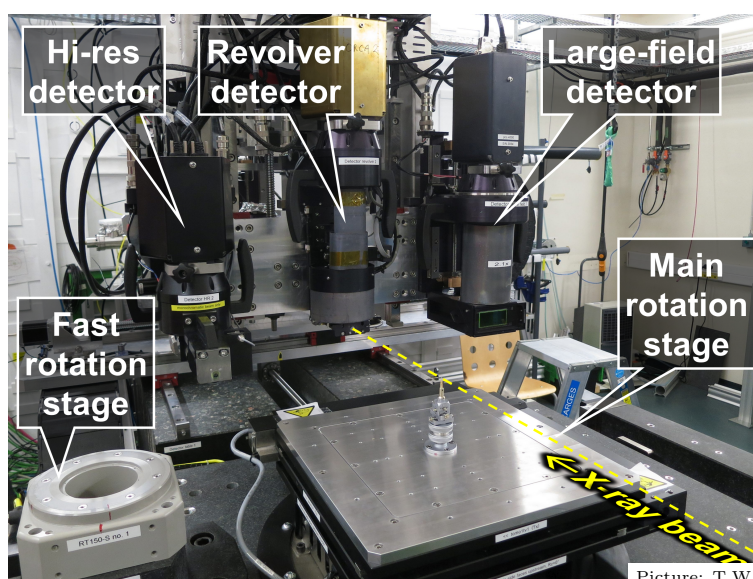
Picture: T.W.

Figure 4.2: Microtomography station 1 of ANATOMIX with sample stage in the foreground and three different detectors on the detector table behind. The sample mounting system installed is the standard one based on a Huber goniometer head (see text).

Table 4.1: Specifications for Huber specimen carrier pins, used for static tomography measurements on free-standing solid samples in microtomography and nanotomography. See Figure 4.3 (center) for illustration.

Product designation	Specimen carrier
Make and model	Huber 1002-18MS
Height	12.5 mm
Outer diameter	3.15 mm
Diameter of central hole	1.5 mm (0.8 mm available on request)
Product web page	https://www.xhuber.com/en/products/4-accessories/ 40-goniometer-heads/head-accessories/specimen-carrier/

drawing of a pin is shown in Figure 4.3 (center). An example of a sample mounted and ready to be measured is shown in Figure 4.4.

The goniometer head having a central mounting hole of around 3.2 mm (1/8"), the standard for many mounts used in X-ray diffraction and scanning electron microscopy. Any cylindrical holder with about 3 mm diameter can in principle be inserted into it as an alternative to the brass pins. In particular, for samples that are larger and in cases where it is not necessary to place the detector very close to the sample, sample carrier stubs for scanning electron microscopy (Figure 4.3, right) can also be used. They are available in a large variety of versions and in different materials.

Another class of alternative holders that are sometimes used for free-standing solid samples on ANATOMIX are wooden shashlik sticks (Figure 4.5). They can be bought in most supermarkets (but make sure the diameter is correct). To get them into shape, you can
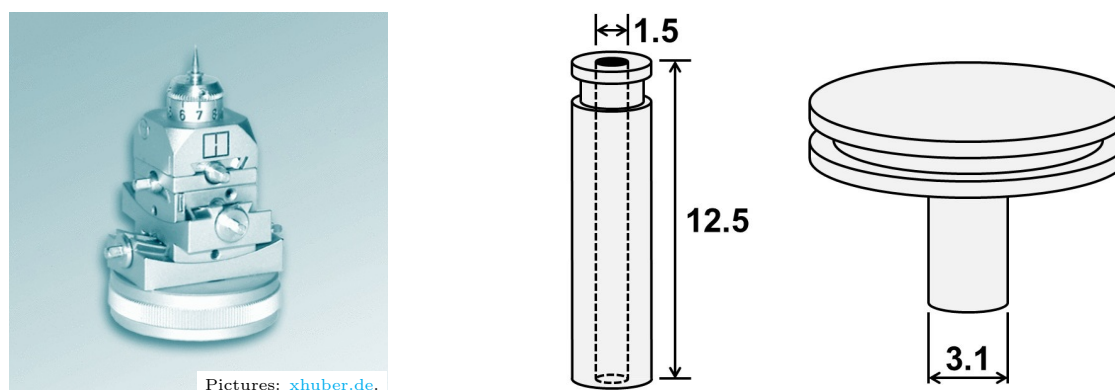

Figure 4.3: Sample mounting system for static tomography on free-standing solid samples. **Left:** Goniometer head model Huber 1005 (available at the beamline). **Center:** Specimen carrier pin, e.g., Huber model 1002-18MS (see Table 4.1 for specifications), commonly used for mounting samples. The hole in the center of the pin may or may not be used for mounting. The brass pin is inserted into the goniometer head from the top. **Right:** SEM stubs can also be used to mount samples on the goniometer head. They are standard components for scanning electron microscopy and available in different sizes from a variety of suppliers. Note, however, that depending on the diameter of their table-top surface, they will impose a minimum distance between sample and detector and are therefore not suitable for high-resolution studies at lower photon energies.
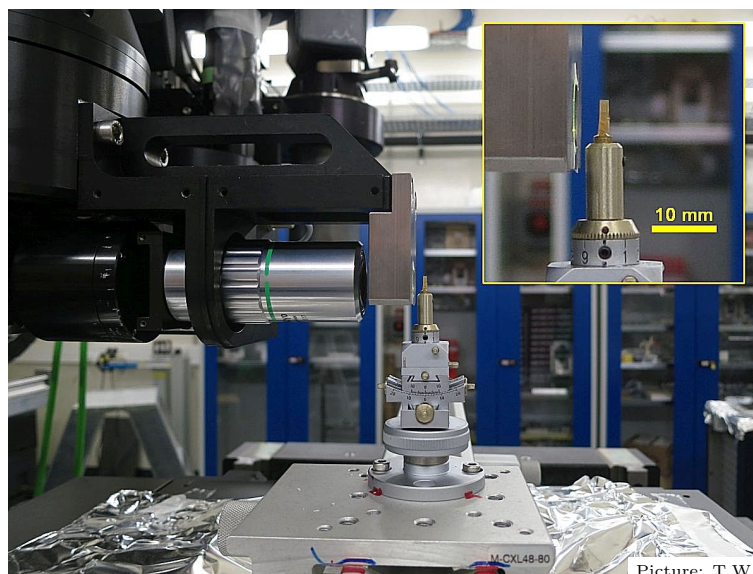
Picture: T.W.

Figure 4.4: Free-standing sample mounted on a Huber brass pin before the high-resolution detector for monochromatic imaging. The inset on the upper right shows an enlarged detail of the sample and its surroundings.

Picture: T.W.

Figure 4.5: Wooden shashlik sticks from the grocery store, such as those shown in this picture, can be used as an alternative to metal sample pins or SEM stubs. Make sure they have a diameter of 3 mm so they fit snugly into the goniometer head.

Figure 4.6: Microcentrifuge tubes exist in different shapes and sizes and can be bought from suppliers of biomedical laboratory equipment.

cut them with a wire cutter and sharpen the end onto which you would like to glue the sample. The wood structure is usually good for gluing, and the internal microstructure of the wood can also serve as a reference to judge data quality.

4.2.2 Samples in a liquid environment

Samples in liquid environments are usually kept in a container that is, in its turn, mounted as a solid, free-standing sample. Containers should generally be made of plastic, not glass (to minimize X-ray absorption by the container). Samples with a diameter of several mm are often kept in microcentrifuge tubes (Figure 4.6) for the measurements. Figure 4.7 shows two examples of samples in liquid, mounted on the ANATOMIX microtomography sample stages in different ways. For smaller samples, pipette tips (Figure 4.8) can be suitable.

In any case, the samples should have sufficient contact to the walls and/or base of the container to be held in place during the measurements with a stability corresponding to a small fraction of the pixel size.

Flat surfaces are easier to fix on another flat surface than rounded ones; be aware of this when you choose your container and the way you put the samples in it. You may prepare samples such that the container is standing "upside down" on its plug or lid, if it has been made sufficiently leak tight.

Note that high-resolution studies on samples in liquids are often made difficult by the formation of bubbles due to X-ray-induced hydrolysis during the scan. If bubbles appear during a scan, the data are usually unusable. This risk is generally high in studies with a spatial resolution corresponding to submicron-size pixels. Do not hesitate to discuss this question with the beamline staff.

4.2.3 Samples for TXM nanotomography

For nanotomography using the transmission X-ray microscope, samples have to be particularly small and at the same time mounted so that they allow unobstructed transmission
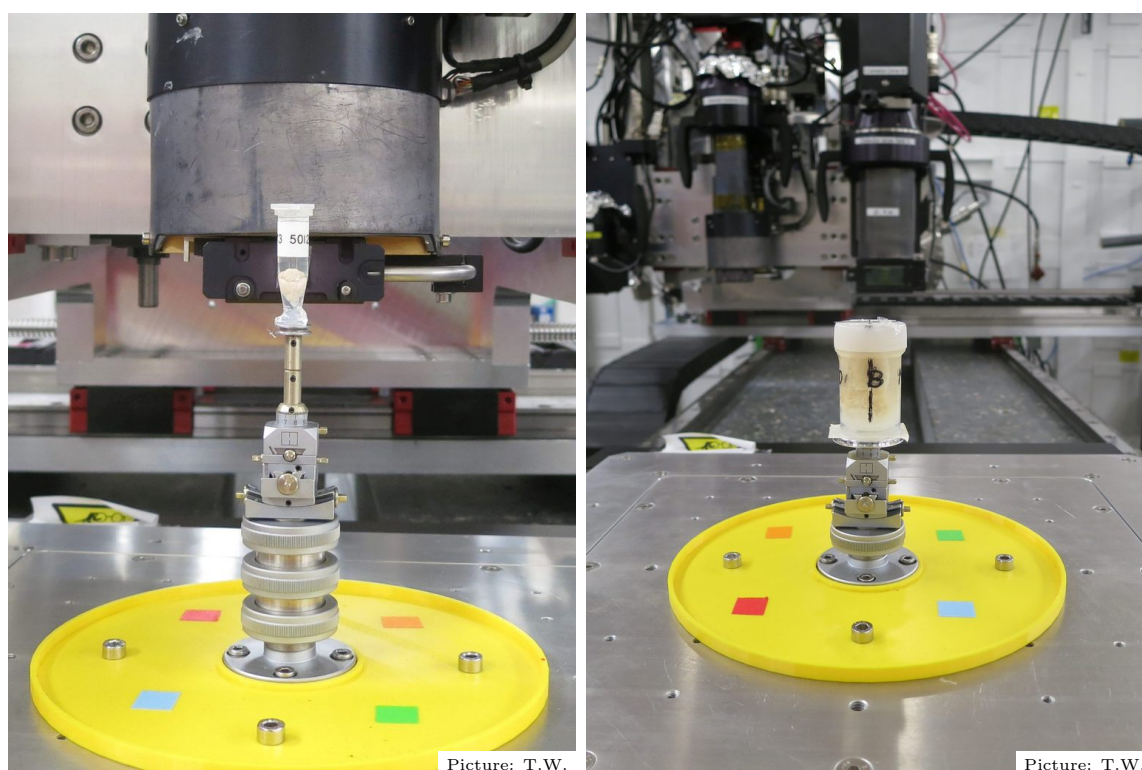
Figure 4.7: Biological tissue samples in liquid environment mounted on the ANATOMIX microtomography sample stages. **Left:** mouse brain in liquid inside a microcentrifuge tube. **Right:** bone biopsy inside a plastic container. Note that in this example, where the instrument resolution was relatively moderate with a pixel size of 3.1 µm, the container was simply held in place by a strip of double-sided adhesive tape on an SEM stub, the stub itself remaining in place on the microtomography stage between sample changes.

of the X-ray beam over the full rotation range of 360°. Details will depend on each specific project. Sample preparation and mounting should be discussed in detail as soon as possible with beamline staff.

4.2.4 Samples requiring precise tilt alignment

A small number of experiments require precise tilt alignment of each sample in the X-ray beam prior to data acquisition. For microtomography, ANATOMIX offers a pair of motorized tilt stages (model 5202.60, Huber Diffraktionstechnik, Rimsting, Germany) that can be used to add motorized tilt control to the usual motorized XYZ translation alignment axes. This option is not part of the standard sample environment and is available upon request prior to the experiment (so far only on microtomograph 2 in hutch EH4). Note that the available vertical space between sample mount and beam position is considerably reduced when using the motorized tilts, and that the central hole in the sample stage is not usable when the tilt stages are used. Figure 4.9 shows pictures of the sample stage in standard configuration and, respectively, with the motorized tilt stages mounted.

Picture: Nadina Wiórkiewicz (Nadine90) / Wikimedia Commons; license: CC-BY-SA 3.0.

Figure 4.8: Pipette tips can be suitable containers for smaller samples in liquid.
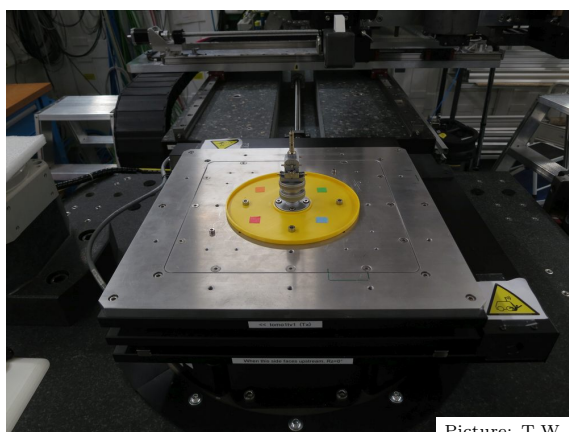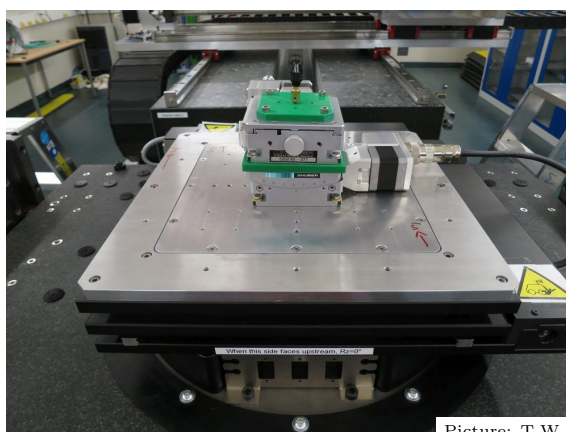
Picture: T.W.   Picture: T.W.

Figure 4.9: Microtomography sample stages in different configurations. ***Left:*** standard configuration with Huber goniometer head. Other sample mounts than the Huber head can be used. ***Right:*** motorized tilt stages added (option available upon request). The drill-chuck style mount can be replaced by a goniometer head or other sample mounts.

Figure 4.10: External hard disk remain the preferred way of transferring tomography data from ANATOMIX to users' home laboratories. *Left:* USB 3.0 disk with flat USB-A connector. *Right:* SATA disk in docking station (docking stations are available at the beamline).

4.3   Other things to provide

4.3.1   Hard disks for your data

The data from a tomography experiment of a few days duration typically have a total volume between several terabytes (TB) and a few dozen TB.

While SOLEIL now has a system that allows you to download your data over the Internet to your home institute (see section 6.1), we currently still strongly advise our users to transfer the data to external hard drives while you are on site for your experiment.

It is therefore necessary that you bring external hard disks with sufficient volume. These can be connected to dedicated PC workstations at the beamline, running under Microsoft Windows 10, to retrieve the data during the experiment and immediately following it.

To be sure that your disks are compatible with our equipment and can be used to download your data, make sure they respect the following:

- **Disks can be "naked" SATA disks or have USB 3.0 connectivity** and a cable with a standard USB-A flat connector (Figure 4.10). USB 2 is practically impossible to use because of its totally insufficient data transfer rate.

- **Make sure that all disks you bring have been formatted in NTFS format and tested by you before the experiment.**

  - Some formats, e.g., exFAT, will allow read/write but at a drastically reduced speed (10× slower than normal, around 10 MB/s instead of $\gtrsim$ 100 MB/s), making them basically unusable for data transfer during the experiment. Be sure you check the format of your disks before your beamtime, and re-format them into NTFS if they are in a different format.

    – Note that there are hard disks, including from well-known suppliers, that require using the manufacturer's proprietary software and administrator rights on the formatting computer to be formatted. Since we do not have administrator rights on our data transfer PCs, you may not be able to format your disks in this case, if you haven't done it at home before the experiment.

- **Storage solution that rely on network connectivity, such as network-attached storage (NAS) systems, are not suitable.**

Necessary disk capacity   The disk space needed for the data from an experiment will depend on the number of tomography scans, their dimensions and a few other parameters. Generally, the raw data require 2 bytes per pixel in each image (as they are composed of 16-bit unsigned integer values), whereas the reconstructed volume data, which are in 32-bit float format, require 4 bytes per voxel.

For the typical case of a tomography scan acquired with the beamline's Hamamatsu Orca Flash camera in full-frame unbinned mode (2048×2048 pixels, i.e., 4 Megapixels per frame, corresponding to 8 MByte) and 2000 projection angles per scan, the raw data amount to approximately 16 GByte (= 2048×2048 pixels $\times\, 2$ bytes per pixel $\times\, 2000$ projections). (In reality it is a bit more because there are also reference images acquired with a scan.) The reconstructed volume has $(2048)^3$ voxels of single-precision float type, i.e., 8 Gigavoxels $\times$ 4 bytes/voxel, i.e., 32 GB. So the total size on disk of such a scan is 48 GB.

In the less typical, but possible case where the Orca Lightning camera is used instead of the Flash, with a region of interest of 3000×2400 pixels and in extended-field (=offset) scan mode with 8000 projections and a reconstructed volume of 5600 voxels diameter, the raw data per scan will amount to 110 GB and the reconstructed volume to an additional 280 GB, i.e., total size on disk 390 GB per scan.

For standard tomography scans, the total size (raw data plus reconstructed volume) on disk for a number of n_s tomography scans, in terabytes, is approximately

$$\frac{6 \times n_s \times n_x^2 \times n_z}{10^{12}} \, , \tag{4.1}$$

where n_x, n_z are the numbers of detector pixels in the horizontal and, respectively, vertical dimension.

An "extended-field" scan (i.e., scan with off-center rotation axis to increase the effective reconstructed region) will typically require 4 times more space than a standard scan with the same detector configuration.

On the other hand, acquisitions with a binned detector or a region of interest (ROI) set on the detector will result in correspondingly smaller data. 2×2 binning will typically gain you a factor of 8 in the total disk size the scan requires.

If volume reconstructions are performed with more than one method or parameter set for each scan (e.g., a standard reconstruction plus a Paganin-filtered reconstruction), then size required by the additional reconstructed volumes must of course also be taken into account.

Picture: Andrés Nieto Porras; license: CC-BY-SA 2.0.

Figure 4.11: Coffee capsules of the type used at ANATOMIX (not included in scope of service).

The minimum necessary disk capacity you should provide is then obviously the size per scan multiplied by the number of scans you hope to be able to acquire. It is a good idea to apply a safety margin (factor of 2 or similar) to this estimation.

If the estimation above seems too complex, a simple rule of thumb is to bring disk capacity of **10 TBytes per day of beamtime.**

4.3.2 Coffee, soft drinks and other stuff to keep you going

There is no store on or near the SOLEIL site, and aside from the laboratory restaurant for your meals and a few vending machines you will not easily be able to buy anything, so think of bringing along what you need.

A coffee machine for Nespresso-based capsules (Figure 4.11) is available in the meeting room of the beamline. Unfortunately SOLEIL cannot provide capsules, so we kindly ask you to bring your own. Be sure to choose standard Nespresso (or compatible) capsules, not capsules of the "Nespresso Vertuo" system.

Cups and glasses are available at the beamline. We kindly ask you to clean up and stow away all dishes right after use. Also please wipe dry all steel surfaces in and around the sink immediately after use, to avoid water stains.

A food fridge is also available, but it is small and primarily intended for soft drinks. In any case, please make sure to leave no items in the fridge after your experiment.

4.4 Shipping things to ANATOMIX

If you need to send material to ANATOMIX, please use the following address scheme for shipping:

> Synchrotron SOLEIL
> Beamline ANATOMIX – *⟨Name of your local contact⟩*
> L'Orme des Merisiers
> Départementale 128
> 91190 Saint-Aubin
> France

If you need to supply a telephone number for shipment, please see Table 3.1 on page 13 for the beamline scientists' numbers.

Never send us any goods, especially samples, without prior agreement. Before shipment, you should discuss the details with your local contact. Also let him/her know once you have sent the parcel out, and provide relevant information (tracking details, picture of parcel, etc.).

Chapter 5

While you are at SOLEIL and ANATOMIX

5.1   When arriving

$\longrightarrow$ *For general information on how to get to SOLEIL, see the web page* Come to SOLEIL *and/or an online map service, for example* OpenStreetMap.

When you have arrived at SOLEIL and passed the site admission procedure, aside from checking in at the Guest House, the first thing to do is usually to go to the beamline control room and/or call the local contact of your experiment. During office hours, he is likely to be already at the beamline (phone +33 1 69 35 97 31).

Cell phones   Please note that the signal for mobile telephones is particularly weak in the ANATOMIX user zone. You will most likely not be able to receive or make calls with your cell phone while you are at the beamline. You will also probably not be able to reach your local contact or anyone else on the beamline on their mobile phones. Use the land lines of the beamline to call people there.

Finding the ANATOMIX beamline   The ANATOMIX user zone (experimental hutches, control room etc.) is located in a 150-m-long extension building sticking out essentially westward from the main synchrotron hall (Figures 5.1 and 5.2). To get there, once in the synchrotron hall, you can either

- walk clockwise and turn left into the extension building after passing the ROCK beamline (path indicated by the green dashed line in Figure 5.1), or

- walk counterclockwise (orange dashed line in Figure 5.1), turn right into the extension building after passing the DIFFABS beamline, then walk past the NANOSCOPIUM beamline until the very end of the extension building and around the big green hutch EH4 (Figure 5.2), or

- enter the building through the entrance from parking lot P4 (junction of the hall with the extension building, Figure 5.1), then turn left immediately into the long corridor leading to the ANATOMIX user zone.

29

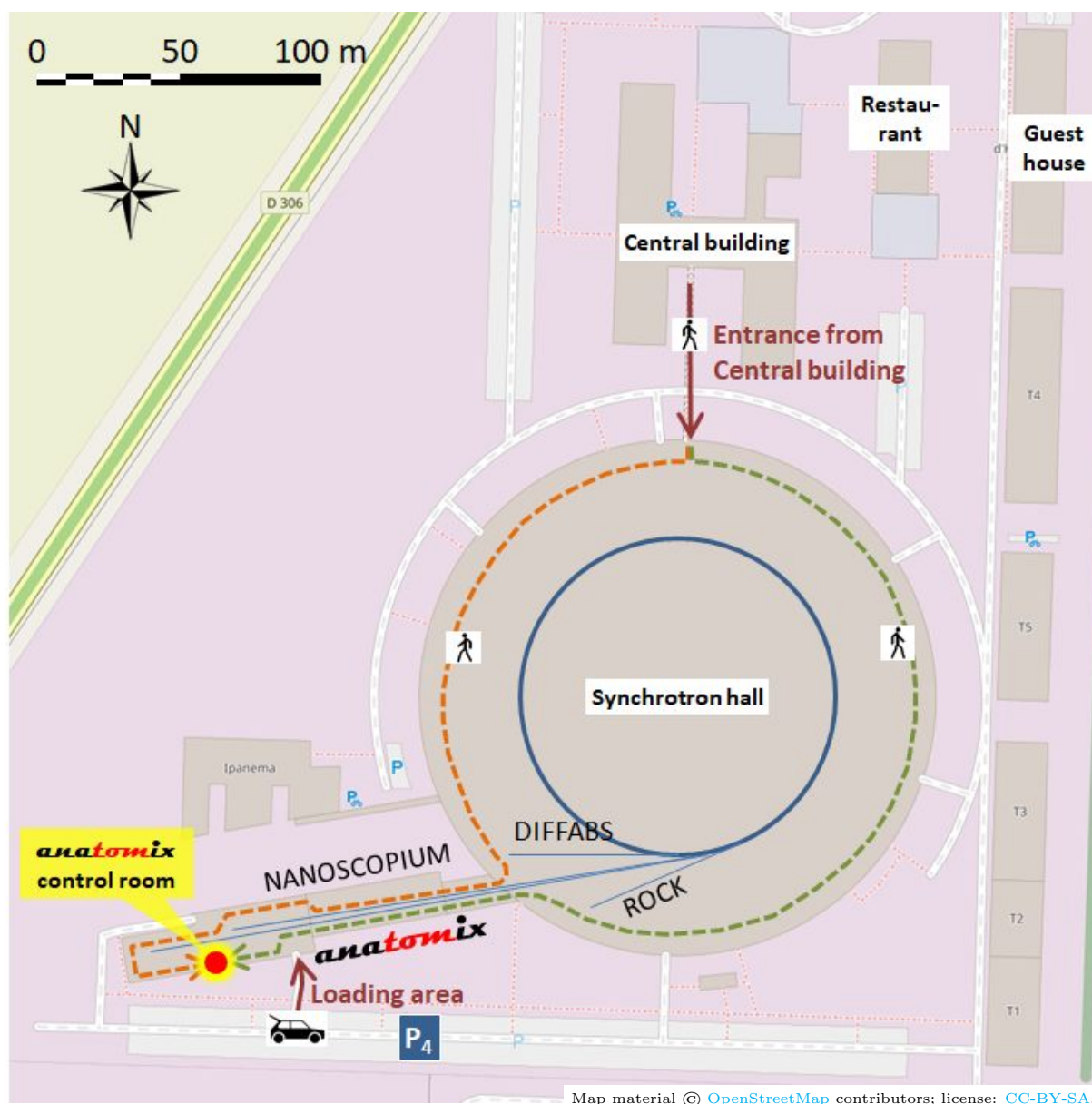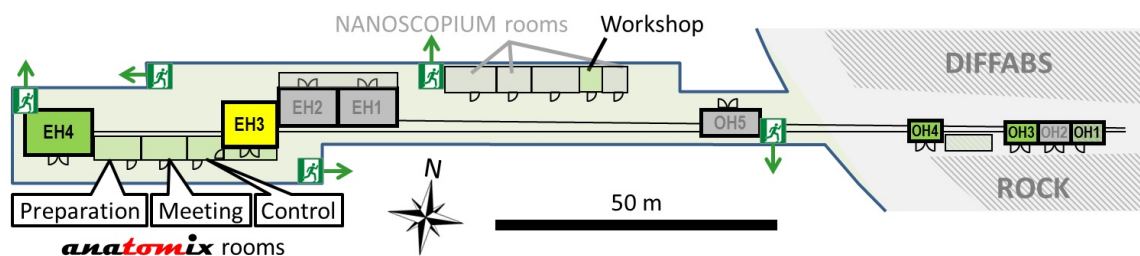**Figure 5.1:** Getting to the ANATOMIX beamline (see also text).

Picture: T.W.

Figure 5.2: ANATOMIX beamline floor plan. On the right, the synchrotron hall. On the left, the extension building for the long beamlines NANOSCOPIUM and ANATOMIX.
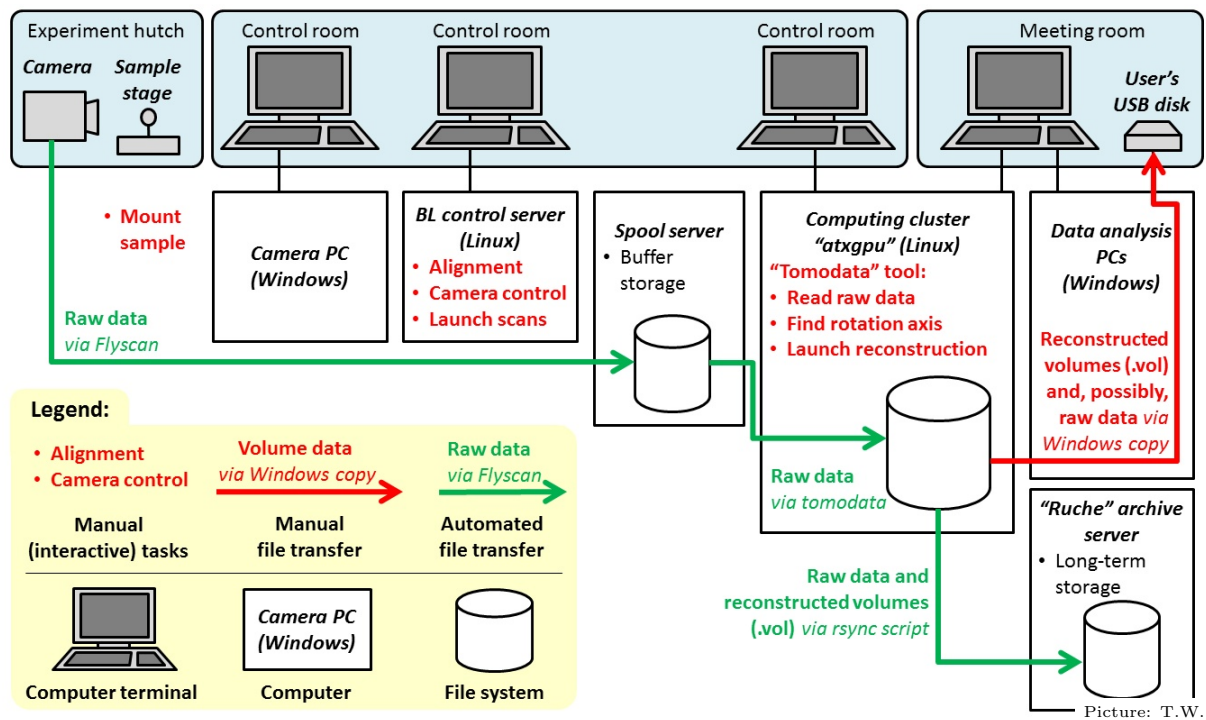
Figure 5.3: Workflow of a typical tomography experiment on ANATOMIX using the standard configuration of the Flyscan architecture. Items written in red ink indicate steps requiring action by the users.

5.2   During data collection

5.2.1   Workflow

Figure 5.3 shows the workflow of a typical (static) tomography experiment on ANATOMIX using the standard Flyscan configuration. (*Flyscan* is the SOLEIL electronics and computing architecture for on-the-fly scans, also known as continuous scans, i.e., scans in which the motorized axes do not stop moving while data are being acquired. The Flyscan architecture enables continuous scans in which the scan axis position and detector trigger are synchronized.)

Standard configuration   In the standard configuration, once the sample has been mounted and aligned and a tomography scan launched, the raw data (mostly projection radiographs, but also flatfield images and dark images) acquired by the camera are directly transferred to an intermediate storage server called the *spool server*, or simply *spool*. On the Linux computers at the beamline, the spool file system is mounted under the path `/nfs/srv3/spool1/`, but you won't really have to access this file system directly yourself. Instead, you control the data processing from a console of the tomography reconstruction cluster "atxgpu" using a text-menu-based software tool named "tomodata". This tool will allow you to select scan data, which it will subsequently read from the spool. It will then allow you to launch the necessary processing steps on these data. These steps usually include finding the exact position of the rotation axis in the acquired projection radiographs and launching the tomographic reconstruction of the full volume.
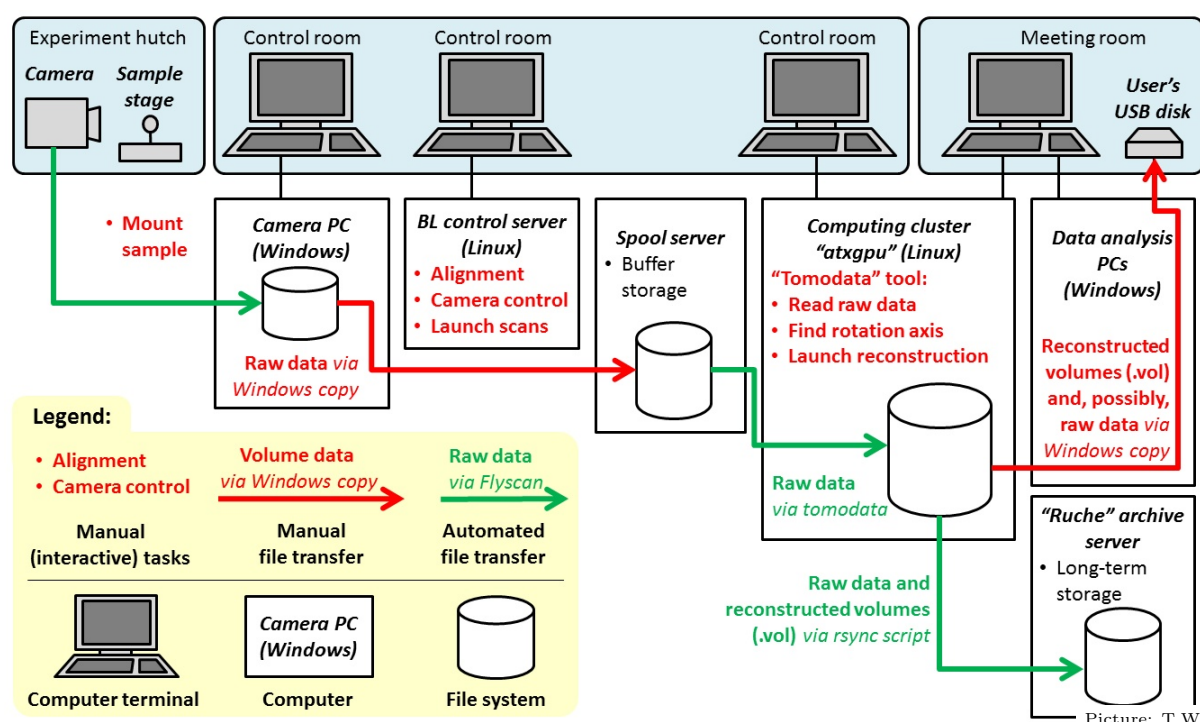
Figure 5.4: Modified workflow in cases where raw data are saved on the internal hard disk of the camera-control computer.

The reconstructed volumes will be written to atxgpu's file system, along with a copy of the raw projection data.

An automatic file copy process (using the `rsync` command), launched by the local contact once at the start of the experiment, will transfer newly-created data on atxgpu (raw data as well as reconstructed volumes and metadata such as the parameter files for the reconstructions) to SOLEIL's central archive server, the "Ruche" ("beehive"). This process does not automatically erase the data from the atxgpu file system.

Modified configuration For some experiments, the standard configuration cannot be applied, because the Flyscan architecture cannot be used and/or because the raw data are not written directly to the spool, but first to the internal hard disk of the computer that controls the detector ("camera PC"). The only major difference in workflow in this case, compared to the standard configuration, is that an additional, user-controlled data copying step is required to transfer the data from the internal hard disk of the camera PC to the spool (Figure 5.4). (In addition, when the Flyscan architecture is not used, the user interface to control the data acquisition will be very different from that of the Flyscan.)

Organizing work Experience shows that the experimentalist who controls the acquisition (changing samples on the instrument, aligning the sample in the X-ray beam, launching the tomography scans) is kept busy doing this and has little or no time to do something else, given that scans typically take only several minutes. A second experimentalist is usually also fully absorbed by taking care of the reconstructions. And somebody needs to

Table 5.1: Example of how work can be divided between three experimentalists.

Experimentalist A (Acquisition)	Experimentalist B (Reconstruction)	Experimentalist C (Samples and data transfer)
Acquire scan #1: • Mount sample • Align sample • Launch tomo scan		
Once acquisition of scan #1 finished:		
Acquire scan #2: • Mount sample • Align sample • Launch tomo scan	Process scan #1: • Select and read data • Find rotation axis • Launch reconstruction of full volume • Inspect result • If needed, refine parameters and re-launch	*Throughout experiment:* • Prepare samples • Manage data retrieval to external hard disks: launch copies, keep a list etc.
Once acquisition of scan #2 finished:		
Acquire scan #3: • Mount sample • Align sample • Launch tomo scan	Process scan #2: • Select and read data • Find rotation axis • Launch reconstruction of full volume • Inspect result • If needed, refine parameters and re-launch	

take care of providing new samples and of managing and monitoring the data transfer to your hard disks as more and more data pile up.

Dividing work among the people present for the experiment is therefore highly recommended, if not indispensable. Table 5.1 shows a typical way of sharing the work if the experiment is sufficiently staffed to have three people present at all times.

5.2.2 Copying data to your hard disks

How to copy   To retrieve your data toward the external hard disks you have brought, you will take advantage of the fact that atxgpu's file system is directly accessible with a fast connection from the three "data PCs" operating under Windows 10. Their consoles are located in the beamline meeting & data room (Figure 5.5). Thus, you can simply connect your disk(s) to the green USB-3.0 extender boxes and use the Windows copying procedure to copy your data from the cluster to your hard drive. The atxgpu file system is mounted on the Windows PCs as a network drive named "`homes ATXGPU`". To go there, open a Windows Explorer window (for example, by clicking on the folder icon in the left part of the taskbar at the bottom of the screen). The drive "`homes ATXGPU`" should be one of the many entries in the navigation pane on the left of the Explorer window. Open this drive, then go to the subdirectory `proposal`. From there, go to the subdirectory

Pictures: T.W.

Figure 5.5: Facilities for retrieving data. **Left:** One of the 3 data PC consoles in the ANATOMIX meeting & data room. **Center:** USB extenders on a console. The black box on the left is a USB-2 extender, not suited for data transfer to your hard disks because it is too slow. The smaller green box is the USB-3.0 extender for data transfer. **Right:** Dock for SATA disks, an alternative to USB disks.

whose name corresponds to the current year, and then to the directory corresponding to your proposal. Figure 5.6 shows an example screenshot of a Windows explorer window.

Don't wait! A typical tomography experiment will produce several terabytes of data per day of beamtime. These need to be copied to the external hard disks you have brought.

As already mentioned in section 4.3.1, we advise you to buy and bring USB-3.0 disks. While the USB 3 standard theoretically allows for data transfer rates up to 640 MB/s, the transfer rates we observe typically range between 40 and 100 MB/s. In other words, each
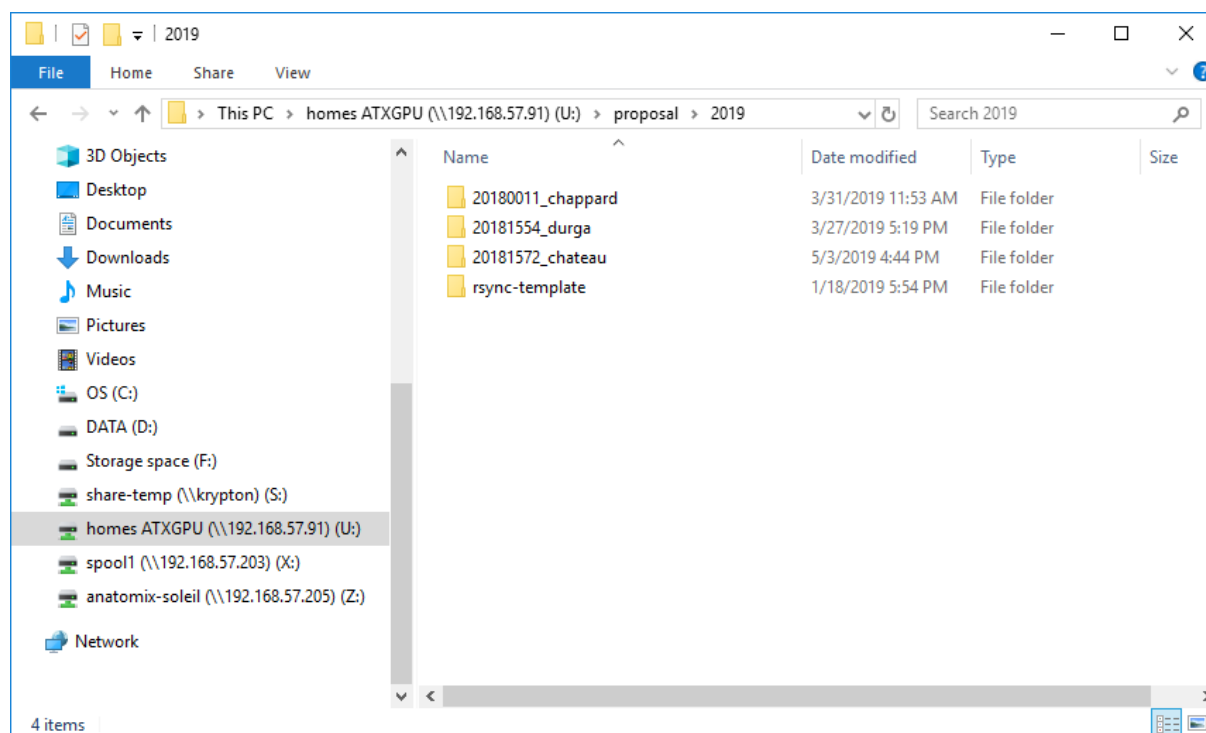
Figure 5.6: Screenshot of a Windows explorer window on one of the data PCs in the ANATOMIX meeting & data room, showing where to find the atxgpu cluster's file system on these machines.

terabyte of data will take between 3 and 7 hours to transfer. This means that transferring your data to your disks is not much faster than producing the data.

You should therefore start transferring the results to disks as soon as the experiment is running smoothly and has produced the first reconstructed data of good quality.

Chapter 6

After the experiment

$\longrightarrow$ *See also the page* After the experiment *on the SOLEIL web site for more general information.*

6.1   Retrieving your data with Globus

> **Warning: Data retrieval from SOLEIL via Globus is currently not stable, and the beamline staff cannot give support in case of problems. We strongly recommend against relying on Globus as the only means of retrieving your data.**

If you have not copied your data to external hard disks during the experiment (section 5.2.2), you have the possibility to download them via the Globus system implemented at SOLEIL. To do this, the following conditions must be fulfilled:

- The data to be transferred must have been copied to the Globus filesystem by your local contact;

- You have an ORCID account or an institutional account that can be used with Globus;

- You have a sufficiently fast Internet connection to perform the download in reasonable time.

Globus is accessible from within the SUNset (log in to SUNset, then select tab "Experiment Data"). A step-by-step guide on how to use Globus (PDF file) is also available; you can download the latest version of this manual from the same location in the SUNset.

6.2   Remote access to data processing

It may happen that you realize after returning home that you should redo some of the tomographic reconstructions, or that there a few scans that you forgot to reconstruct, etc. Since our reconstruction pipeline is not made to be deployed on external computers, this

will require that you access our computers, which is best done remotely (unless it is easy for you to come to SOLEIL physically). It is possible to log in remotely to SOLEIL if we agree on the dates and times, and if we grant you the authorizations in the agreed time period to log in to our systems from your home institute. If you need this type of remote access, please get in touch with us.

6.3   Publication of your results

When publishing results that have been obtained using data acquired at SOLEIL and in particular ANATOMIX, we kindly ask you to follow a few guidelines laid out below and respect all the points.

Contact us while your manuscript is still in progress. It is not nice for beamline staff to find out by chance on the Internet that someone has published data from an experiment performed on their instruments. It is also not nice when a paper gives inaccurate details about the experimental setup, or when authors have acknowledged their own funding agencies, but not those that financed the beamline and the equipment that the authors used to obtain their data. Unfortunately, all of this has already happened, and it sometimes causes frustration or even resentment. Therefore, please contact us in the writing phase of your manuscript so that we become aware of your publication project and can interact with you.

Credit beamline staff. There are two alternative ways to give credit to the beamline staff involved in your experiment:

1. If you feel that the role of the local contact and other beamline staff remained within the scope of what can be reasonably expected in terms of level of support (i.e., beamline preparation, introduction into operation and then daytime availability in case of problems, with on-call duty till late evening), the right way is to mention the beamline, proposal number(s), and acknowledge assistance from SOLEIL beamline staff and/or each person for their help. A model phrase can be found on the SOLEIL web page *After the experiment*.

2. If, on the other hand, you feel that the beamline staff's contributions went beyond their obligation, and/or if you would like a beamline scientist to contribute to parts of the paper (e.g., to the "Methods" section of the manuscripts), then you can ask those persons whether they would like to act as co-authors.

Acknowledge our funding agencies and programs. Since the construction of ANATOMIX was funded by a big grant from the French State without which the beamline would not exist, and since we also received smaller grants for some of the equipment, we ask you credit our funding bodies and programs properly. Thus, for all publications with results from ANATOMIX, you should add the following statement in the acknowledgments section:

In addition, if you have used the TXM with the direct-coupled fiber detector, you are also requested to acknowledge the co-funding of this detector. The phrase required is:

> "This work was supported by the Paris–Ile-de-France Region, via the network of excellence DIM RESPORE."

Cite beamline reference paper. If you want to cite a reference on the beamline, please do not cite this guide but a suitable article in a scientific journal, for example,

- for details on the microtomography station:
  Weitkamp et al. (2022), doi:10.1088/1742-6596/2380/1/012122

- for details on the TXM nanotomography station:
  Scheel et al. (2022), doi:10.1088/1742-6596/2380/1/012045

- for the beam-steering optics:
  Weitkamp et al. (2017), doi:10.1088/1742-6596/849/1/012037.

,

Send us a reprint. Please send a reprint of your paper to the beamline staff (e.g., by e-mail to your local contact) and the SOLEIL library and enter the bibliographic data into our online user management system, *SUNset*. The SOLEIL web page mentioned at the head of this chapter gives detail instructions on the procedure.

Chapter 7

Technical details

7.1 Detectors

To record X-ray images down to submicron resolution, ANATOMIX uses the concept of indirect detection, in which the X-ray image is first converted to visible light by a fluorscent screen, or "scintillator", and then the visible-light image is projected onto the sensor of a scientific-grade digital camera (CMOS or CCD) with visible-light optics.

Thus, in microtomography, the effective pixel size of the images is the physical pixel size of the camera, divided by the optical magnification achieved through the visible-light optics between the scintillator and the camera.

(In TXM nanotomography, the effective pixel size is the physical pixel size of the camera divided by the product of the optical magnification of the visible-light optics in the detector and the X-ray magnification of the TXM.)

Table 7.1: Digital sensors for microtomography at ANATOMIX. ADC: analog-to-digital converter; SNR: signal-to-noise ration; QE: quantum efficiency.

Model	ORCA Flash 4.0 V2	ORCA Lightning	Dhyana95 V2	Dimax HS4
Manufacturer	Hamamatsu	Hamamatsu	Tucsen	PCO
Sensor size (pixels)	2048×2048	4608×2592[b]	2048×2048	2000×2000
Pixel size (μm)	6.5	5.5	11.0	11.0
Max. frame rate (fps)	50 ; 100[a]	30	24	2277
Exposure times	40 μs to 10 s	50.4 μs to 1 s	21 μs to 10 s	1 μs to 40 ms
Max. frame buffer	Disk size[c]	Disk size[c]	Disk size[c]	36 GB
ADC Bit depth	16	16	16	12
Max. SNR	37 000	17 000	31 600	1600
Peak QE (%)	82	60	95	47

[a]When using "rolling shutter"

[b]Camera is always mounted in landscape orientation. We recommend limiting the ROI to no more than 3000×2400 pixels to avoid distortion effects.

[c]Frame buffer is limited by the size of the camera PC's internal hard disk

Table 7.2: Types of lens-based detector optics available at ANATOMIX. Note that the "revolver" optics has an objective turret with place for 4 objectives; the turret can be remotely operated. The HR and LF optics require manual intervention to change magnification, which is not usually advised during an experiment. The HR optics can be used with faster and higher-resolving lenses than the revolver but its use is limited to the monochromatic beams.

Name	Revolver (RV)	Hi-res (HR)	Large field (LF)
Type	Microscope	Microscope	Macroscope
Lens type	Mitutoyo microscope lenses	Mitutoyo microscope lenses	Hasselblad photo objectives
Magnifications	$(2\times)$, $5\times$, $7.5\times$, $10\times$, $20\times$ SL	$5\times$ HR, $10\times$ HR, $20\times$, $50\times$ HR	$(0.28\times)$, $0.48\times$, $1\times$, $2.1\times$, $(3.6\times)$
White beam allowed?	Yes	No	Yes

Different models of digital cameras are used at ANATOMIX to cover a wide range of performance parameters in terms of speed, size of the pixel array, and dynamic range. And different detector optics are available to cover a wide range of magnifications with good efficiency.

Table 7.1 gives a list of the available digital cameras, Table 7.2 one of the available detector optics. All cameras can be combined with any of the optical systems, with the exception of the ORCA Fiber camera, which uses a fiber-taper optical system permanently integrated into the camera.

The main detector tables in the two experimental hutches each have four positions for detectors that can be simultaneously mounted; three of those positions are located at the front of the detector carriage and one further downstream. Figure 4.2 on page 18 shows a configuration in which the front positions are occupied, from left to right, by an HR, an RV and an LF detector. Figure 4.4 (page 18) shows the HR detector with a sample in front.

The revolver (RV) detector has parts protruding beyond the scintillator plane, which limits the proximity between sample and scintillator for samples (or sample environments) that are too high. Figure 7.1 shows a profile plan of the RV optics with the relevant dimensions.

7.2 Microtomography sample stages

7.2.1 Dimensions and mechanical interfaces

If you would like to adapt a specific sample environment to our stages, the schematic and dimensions in Figure 7.2 may help you. They provide details of the mechanical interface on which sample environments can be mounted.

For cases in which even the top XY stage needs to be dismounted (only after explicit prior agreement of the beamline staff and if absolutely indispensable), Figure 7.3 shows the interface of the RT500 rotation table after removal of the XY stage and slip ring.
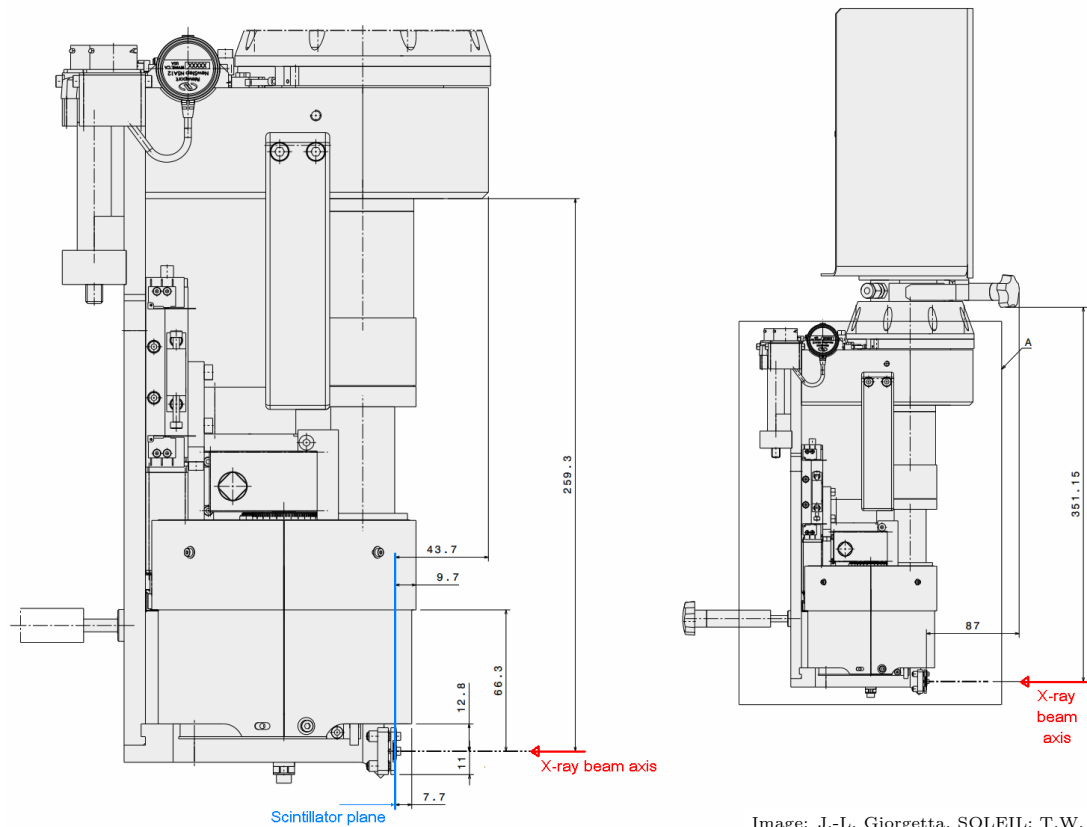
Image: J.-L. Giorgetta, SOLEIL; T.W.

Figure 7.1: Side view of the revolver detectors at ANATOMIX. The X-ray beam propagates from right to left. *Left:* lower part of the optics, not showing the camera mounted. The scintillator plane position is indicated in blue. *Right:* full view with a camera mounted (note that different camera models have different dimensions).
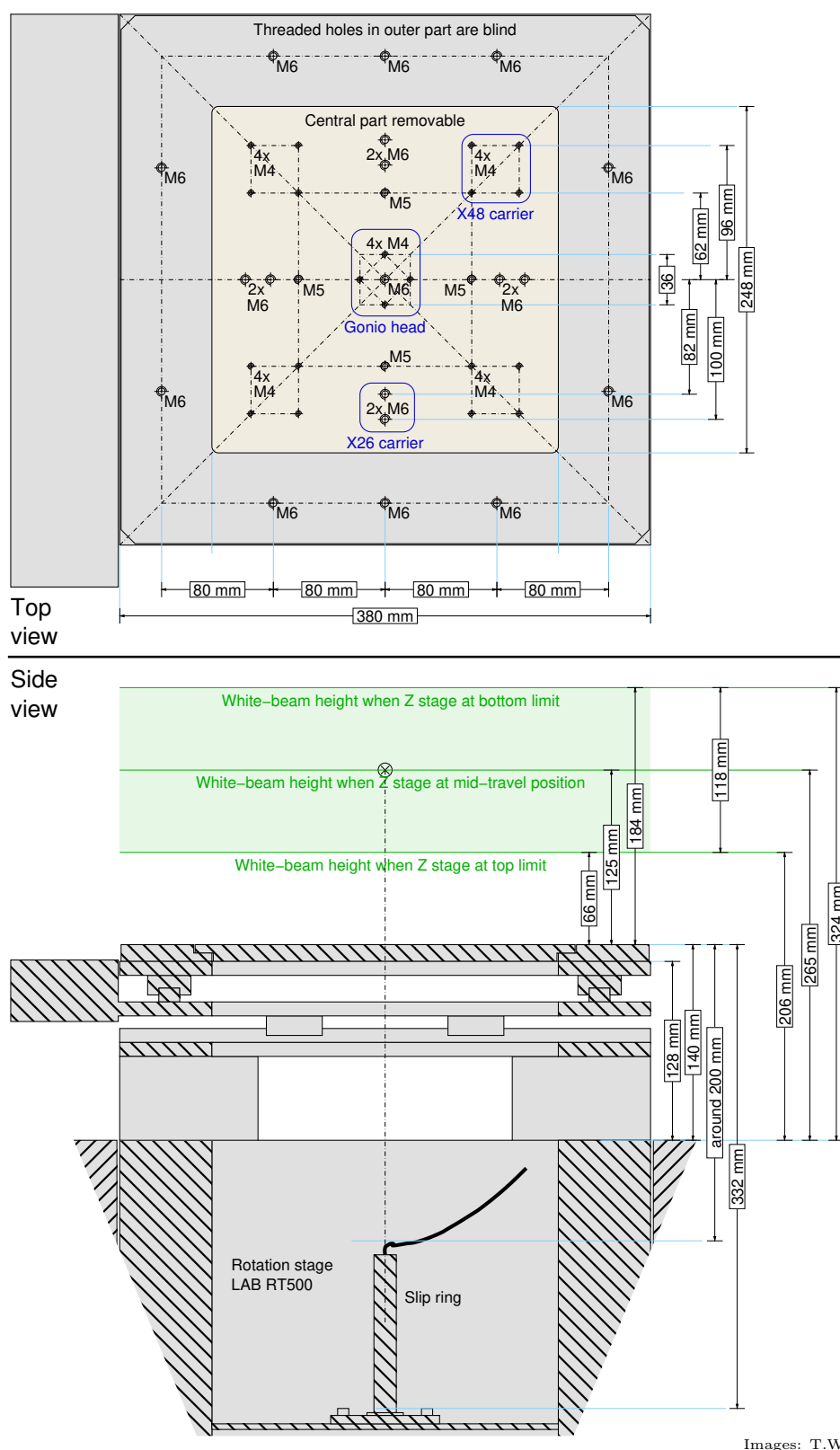
Figure 7.2: Mechanical interface of the microtomography sample stage in EH 3. The sample stage in EH 4 is identical, but the beam height may be slightly different. The monochromatic beam (not indicated in this schematic) is (20±5) mm above the white beam. All threaded holes shown in the top view are available for user experiments.
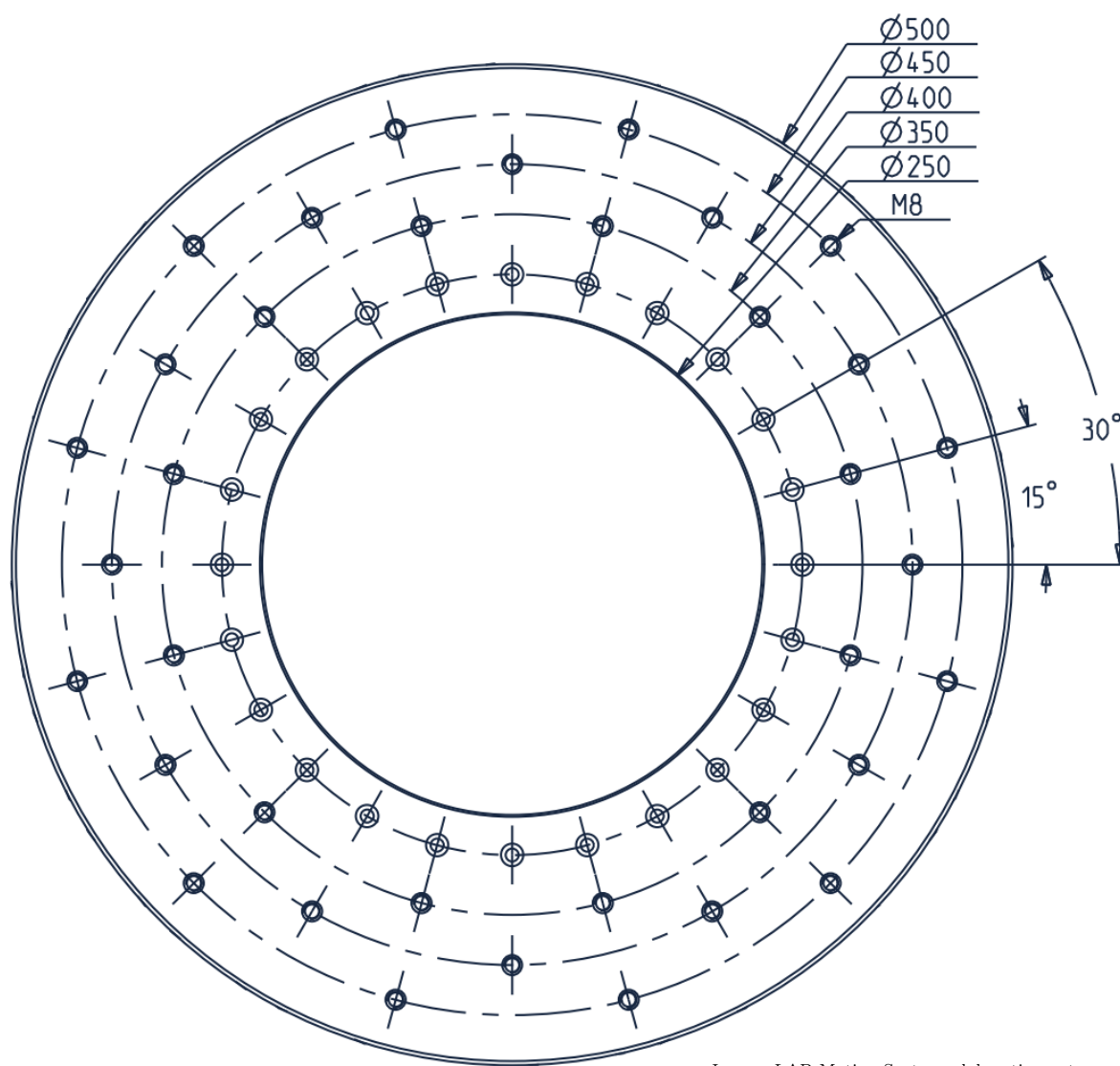
Image: LAB Motion Systems, labmotionsystems.com

Figure 7.3: Top interface of rotation stage LAB RT500 when the XY stage is dismounted (configuration not available for standard experiments).

7.2.2   Slip ring and electrical interface

Each of the large, 50-cm-diameter rotation stages model LAB RT500 on the two microtomography sample stages (microtomograph 1 in hutch EH 3 and microtomograph 2 in hutch EH 4) is equipped with a *slip ring,* i.e., a rotary electromechanical interface that can be used to transmit electrical signals and/or power from the stationary base of the stage to whatever is mounted on top of the rotation stage. Each slip ring has 56 wires. 24 of these are used for the XY translation stages that are mounted on top of the rotary stage.

The remaining 32 wires are available for user equipment (see exceptions below). They are accessible via three 15-pin D-sub (DA-15) connectors. The connectors on top of the rotating stage are female, those on the patch panel at the base of the microtomograph (stationary side) are male. Table 7.3 gives the wiring scheme; Figure 7.4 shows pictures of the connectors.

If you use the motorized sample tilt stages (section 4.2.4), the number of free wires will be considerably smaller because each of the two cradle stages occupies one of the connectors, leaving only the third one free.

Caution: While each wire is specified for a maximum current of 2 A, note that the connectors are absolutely unsuitable for power or voltage levels that can be harmful to people. For example, 230-volt or 110-volt AC power must never be transmitted via these connectors.
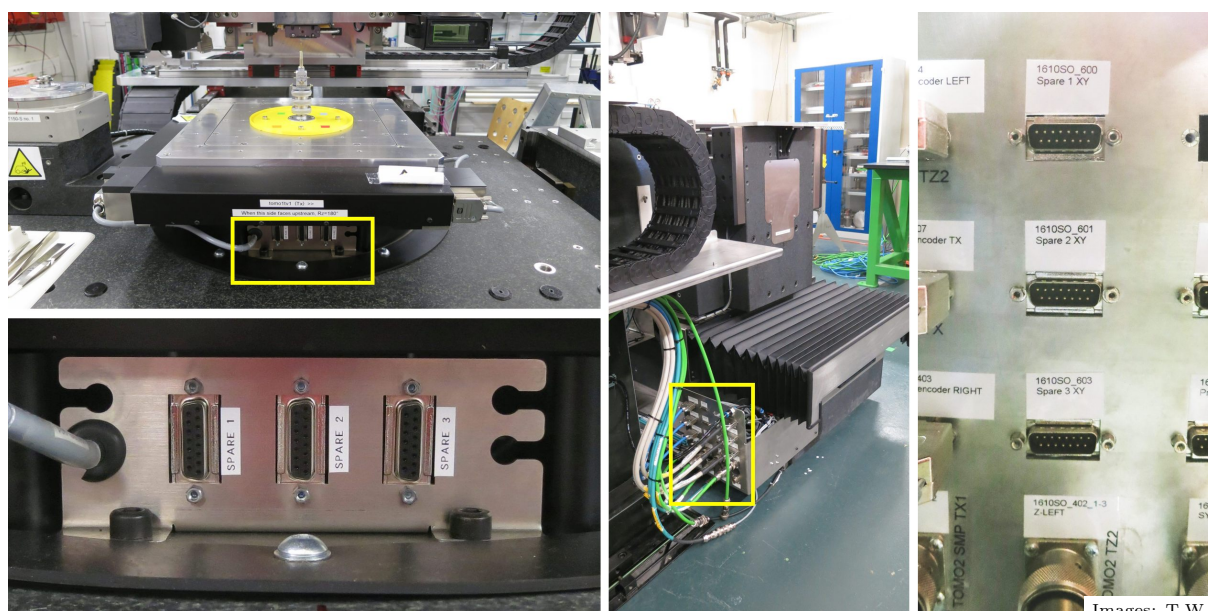
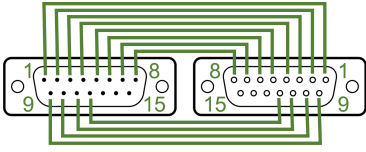**Figure 7.4:** Connectors for free slip-ring wires of the microtomography rotation stages RT500. ***Top left:*** view of the rotation stage; the connectors are marked by a yellow rectangle. ***Lower left:*** closeup view of the connectors on the rotating part of the stage. ***Right:*** patch panel at base of microtomography stage (stationary side; marked by yellow rectangle). ***Far right:*** closeup of the patch panel.

Table 7.3: Usable free wires on the electrical slip rings of the microtomography sample stages 1 and 2 (located, respectively, in hutches EH 3 and EH 4). The schematic on the right shows the pinout and wiring scheme. Note that the connectors on the rotary side are male, while those on the stationary side (patch panel) are female.

Connector label	Usable pins MT 1 (EH 3)	Usable pins MT 2 (EH 4)
"Spare 1"	$\#1, \ldots, \#12$	$\#1, \ldots, \#12$
"Spare 2"	$\#1, \ldots, \#12$	$\#1, \ldots, \#12$
"Spare 3"	$\#1, \ldots, \#8$	$\#1, \ldots, \#4 ; \#6, \ldots, \#8$

Rotary stage   Patch panel

7.3   Tomodata documentation

At ANATOMIX, users control the tomographic data processing, or tomographic *recon-struction*, i.e., the process that leads to reconstructed slices of the imaged objects, on a console of the tomography reconstruction cluster "atxgpu" using a text-menu-based soft-ware tool named "tomodata". This tool was written by Andrew King at the PSICHÉ beamline of SOLEIL, where it is also used. Andy wrote a documentation to "tomodata" which we include in this document on the following pages.

tomodata.py documentation

Andrew King, PSICHE

Table of Contents

Overview

- Tomodata is an old school text menu driven interface, written in Python, for interacting with tomography data and PyHST2.
- All reconstructions are done by calling PyHST2, either directly or by submitting a SLURM job.
- Tomodata prepares the data for PyHST2. It prepares the parameter file used to launch PyHST2. It can calculate corrections that are input to the reconstruction.
- It supports batch processing to apply workflow to multiple datasets, again, either locally or via SLURM.
- It can be used in a live mode, which will watch a directory and reconstruct the latest datasets as they appear.
- It is currently used at PSICHE, ANATOMIX, and on SUMO (for com-psiche and chevreau accounts).

Structure

- The code is designed to be modular. Internally, there is one Python function for each operation on the parameter file, or for each correction. Therefore, any new functionality is added with a new, independent Python function. The aim of this is robustness and simplicity – we don't break the currently working code by adding new things, and each function does one thing. Each function has a common structure to allow it to be used inside an ipython shell environment, or directly from the command line.
- There is one front-end function ("tomodata.py") which contains the user interface. To add a new function requires writing the function, and adding a few lines to tomodata.py to include it.
- So far, the code has been placed in ~/Python/
- Most of the code is supposed to be completely generic, and independent of the beamline.
- In the home directory, there is a BEAMLINE_PARAMETERS.par file, with some beamline specific info.

Future

- The structure of tomodata is designed such that a graphical "wrapper" could by put on top, to present a more friendly user interface.
- Should adapt to PyHST2_2019b or later to benefit from bug fixes and new features – this may involve moving to Python3.
- Should adapt to PyHST2 reading directly from the nxs files. In this case preprocessing data becomes a simple copy of the nxs from spool to local machine.
- A faster single slice reconstruction.

Workflow

(0) Preprocessing – read nexus from spool, write edfs locally. Read par file from spool, write locally with correct paths.

Functions for normal data, fast series, spirals.

(1) Metadata calculations? – things like setting Paganin parameters, calculation of the rotation axis, calculating ring or movement corrections. Reconstruction of a single slice is used to check validity of data and parameters. This is the main function of tomodata.

(2) Reconstruction of volume – main processing step. This can be on a local machine or on a cluster.

(3) Conversion of 32bit float data from PyHST2 to 8 or 16bit to reduce data size.

Batch processing can involve all or any of these steps.

Installation and operation

Launch tomodata from the experiment directory. This is where the data will end up. "tomodata" is used as an alias to launch the Python function of the same name.

```
[com-psiche@PSICHEGPU Michelin_0620]$ pwd
/psichestockage/experiences/psiche/com-psiche/industry/2020/Michelin_0620
[com-psiche@PSICHEGPU Michelin_0620]$ ls
1_00_    1_07_    1_15_    1_23_    1_31_     2_test2  3_08_    3_16_    3_24_    3_32_    3_tes
1_01__1  1_08_    1_16_    1_24_    1_32_     3_00_    3_09_    3_17_    3_25_    3_33_    3_tes
1_02_    1_09_    1_17_    1_25_    1_33_     3_01_    3_10_    3_18_    3_26_    3_35_    4_00_
1_03_    1_10_    1_18_    1_26_    1_34_     3_02_    3_11_    3_19_    3_27_    3_36_    4_tes
1_03__1  1_11_    1_19_    1_27_    1_35_     3_04_    3_12_    3_20_    3_28_    3_37_    4_tes
1_04_    1_12_    1_20_    1_28_    1_test_   3_05_    3_13_    3_21_    3_29_    3_38_    5_00_
1_05_    1_13_    1_21_    1_29_    2_00_     3_06_    3_14_    3_22_    3_30_    3_39_    5_01_
1_06_    1_14_    1_22_    1_30_    2_test_   3_07_    3_15_    3_23_    3_31_    3_40_    5_02_
[com-psiche@PSICHEGPU Michelin_0620]$ alias tomodata
alias tomodata='python ~/Python/tomodata.py'
[com-psiche@PSICHEGPU Michelin_0620]$ tomodata
```

When it starts, tomodata shows a help screen, which is always available as option "h", or if you hit enter with no command given. There are extra functions which are only shown if you use the option "hh".

As a general rule, when the user is asked for an input, the default option will be shown in square brackets [default option]. If you hit enter without any other input you will get the default option.

To process a dataset

Selecting a dataset / Preprocessing

Choose option "s" to select a dataset from the spool. This will open a file dialog window. The normal spool root directory is set in the BEAMLINE_PARAMETERS.par file. The path to the experiment directory (working directory) is used to find the right sub-directory on the spool. You can always navigate to another directory, e.g. the ruche, a local directory, or a different spool directory.

You need to *double click into* the directory corresponding to the dataset that you want to process.

Click OK, and you will be asked if you want to bin the data. This can be useful for increasing the signal to noise, but it is slow, and the normal answer is no, the default option.

The projection data on the spool are read, and converted into unsigned 16bit edf images for PyHST. The acquisition also saves series of bright and dark reference images. These are read, and used to produce average reference images to correct the projections. The median of the bright images, and the mean of the dark images, is used.

Reselecting a dataset

If you have already preprocessed a dataset, you can select the scan from the working directory using option "n". If a reconstructed slice already exists, it will be dispayed using view_only.py.

If you select a dataset that has already been preprocessed (using "s"), you will be asked if you want to repeat preprocessing.

Next steps

There are many options in tomodata for working with your data. There are even more options available in PyHST. The most common / useful / important ones have been implemented in tomodata.

Rotation axis

This is something that has to be done for almost every dataset, and is used as an example of how tomodata works.

From the main text interface, select option "a" – rotation axis options.

This calls the function rotation_axis.py, with the name of the dataset as an argument. The function is called with the argument interactive=True.

Rotation_axis.py can try to find the rotation axis in several different ways. The default option is [a] – automatic. In this case the function reads the scanname/scanname.par parameters files to get the number of images and the angular step size. It reads the projection at 0 degrees, the projection at 180 degrees, the reference and dark images. These are read from the .edf files in the scanname /scanname_edfs/ folder. The 0 and 180 degree images are flat field corrected, the 180 degree image is flipped left-right, and a correlation (row by row for all rows of the image) is used to find the centre of rotation. The user is asked to confirm the result. If confirmed, the value is used to modify the ROTATION_AXIS_POSITION value in the main parameters file scanname/scanname.par.

Points to note

- We read and write the scanname/scanname.par file.
- Inside tomodata, the rotation_axis function is imported. In this mode, interactive=True is the default.
- If we call rotation_axis.py from outside tomodata (i.e. python ~/Python/rotation_axis.py scanname) the default is for interactive=False. These choices correspond to interactive and batch processing. In both cases, the interactive mode can be set as required, but the default behaviour goes like this.
- In the case above, PyHST2 does nothing – we just update the par file.
- Rotation_axis.py has other options for finding or changing the rotation axis. We can simply apply a new value that we have chosen, we can try to guess the position (based on motor positions and pixel size recorded in the par file), or we can "scan" the rotation axis. In this case we reconstruct a slice a several positions, and compare the results. This is slow, and has been partly superseded by rotation_axis_by_reconstruction.py, option "b" from tomodata.

Visualise / view

To check the validity of the current parameters, we reconstruct one slice from the dataset. This is option "v", which calls reconstruct_and_view.py. As above, it is called in interactive mode. Reconstruct_and_view.py asks the user which slice to reconstruct. By default, the central slice of the dataset is reconstructed. The scanname/scanname.par master par file is read. The START_VOXEL_3 and END_VOXEL_3 parameters are modified to correspond to the chosen slice. The OUTPUT_FILE parameters is modified to scanname/scanname_slice.vol. These parameters are written to a new par file scanname/scanname_slice.par. PyHST2 is then called with this par file as argument. PyHST2 is called via a helper function call_pyhst.py. This allows use to handle differences in how PyHST2 is called on different computers (PSICHE, ANATOMIX, SUMO, - is the code run on the local machine, or do we pass by SLURM srun? etc). The slice is then read and displayed using another function, view_only.py. This shows the slice to the user. By default, the image axes are presented in millimetre units (using the pixel size from the par file) and with absolute values of the sample alignment motor positions (read from the par file). Units can be toggled to pixels.

- This shows the hierarchy of subfunctions, and the attempted principle of splitting up functions to avoid writing the same thing many times!
- Call_pyhst.py is one of the functions which must be adapted when installing tomodata on a new beamline / new system.
- Figures are displayed using pylab, which in turn uses matplotlib.
- Reconstructing one slice with PyHST2 is relatively inefficient. This is perhaps something to discuss with Alessandro Mirone for future improvements. On PSICHEGPU, reconstructing n slices has an overhead of about 20 seconds, regardless of whether n=1 or 1000…

Tomodata subfunctions and options

The following is mostly generated by calling:

```
python ~/Python/myfunction.py –help
```

In general, if you work from tomodata in interactive mode you will be guided through the options. If you want to put them in a script for batch processing, you need to specify the options, or use the defaults. There are a few other functions that do not appear in tomodata, but can be used in a script.

Tomodata functions

angle_offset.py	option "w"
auto_crop.py	option "crop"
copy_parameters.py	option "c"
double_ff.py	option "f"
double_ff_special.py	option "ffs"
half_acq.py	option "d"
"help"	option "h"
"extended help "	option "hh"
launch_reconstruction.py	option "l"

live_preview.py   option "live"

mercedes_movement_correction.py   option "mb"

movement_correction.py   option "m"

nonconstant_rings.py   option "nc"

paganin.py   option "p"

preprocess_all.py   option "s"

preprocess_dimax.py   option "sd"

preprocess_fast.py   option "sf"

preprocess_spiral.py   option "sp"

recad_multi_memmap.py   option "x"

reconstruct_all.py   option "A"

reconstruct_and_view.py   option "v"

remove_spikes.py   option "rs"

roi.py   option "r"

rotation_axis.py   option "a"

rotation_axis_by_reconstruction.py   option "b"

select_name_only.py   option "n"

"toggle units"   option "u"

utopec.py   option "y"

zero_clip.py   option "z"

Tomodata function options

angle_offset.py [-h] [-i INTERACTIVE] [-a ANGLE] scanname

Set the angle offset for a reconstruction

(i.e. if you need to rotate a square section sample in order to align the edges with the edges of the reconstruction)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

                Interactive mode [False]/True

  -a ANGLE, --angle ANGLE

                angle offset

auto_crop.py [-h] [-i INTERACTIVE] [-x XSIZE] [-y YSIZE] [-z ZSIZE]

Crop the reconstruction ROI for a tomo scan

(Centred crop – so you give the size you want, and it crops symmetrically)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

                Interactive mode [False]/True

  -x XSIZE, --xsize XSIZE

xsize of reconstruction

-y YSIZE, --ysize YSIZE

ysize of reconstruction

-z ZSIZE, --zsize ZSIZE

zsize of reconstruction

copy_parameters.py [-h] [-i INTERACTIVE] [-s SOURCE] scanname

Copy reconstruction parameters from one scan to another (ROI,Pag,axis pos)

optional arguments:

 -h, --help   show this help message and exit

 -i INTERACTIVE, --interactive INTERACTIVE

Interactive mode [False]/True

 -s SOURCE, --source SOURCE

name of scan from which to copy parameters

double_ff.py [-h] [-i INTERACTIVE] [-a ACTIVATE] [-t DOTUBES] [-x FILTX] [-z FILTZ] [-s SPIRALSIZE] [-n STEP] [-p PIXELMASK] [--homogeneous HOMOGENEOUS] scanname

Make, activate or deactivate double flatfield ring correction

(makes a double_ff image for PyHST, saved as scanname/scanname_edfs/scanname_ff.edf. The principle is that we make an image which is the average of all the projections. We assume that this image should be smooth, or blurred. Anything sharp is a problem like a spot on the scintillator. We filter the mean image with a 2D median filter. Anything that disappears is used in the correction. A bigger filter removes bigger rings. The homogeneous option assumes that the mean image should be completely homogeneous, and any contrast should be corrected.)

optional arguments:

 -h, --help   show this help message and exit

 -i INTERACTIVE, --interactive INTERACTIVE

Interactive mode [False]/True

 -a ACTIVATE, --activate ACTIVATE

Activate (or disactivate) an existing correction [True]/False

 -t DOTUBES, --dotubes DOTUBES

Special correction for the sCMOS lines (tubes) True/[False]

 -x FILTX, --filtx FILTX

Filter size (x, hor) for correction

 -z FILTZ, --filtz FILTZ

Filter size (z, ver) for correction

 -s SPIRALSIZE, --spiralsize SPIRALSIZE

Spiral acquisition original image size y

 -n STEP, --step STEP Step size when making mean

 -p PIXELMASK, --pixelmask PIXELMASK

Threshold for pixelmask to correct only bad spots (0=no mask)

 --homogeneous HOMOGENEOUS

Homogeneous sample True/[False]

double_ff_special.py

Currently inside tomodata only.

(This builds a double flatfield correction by thresholding the reconstruction to remove all rings, and then forward projecting to make "perfect" projections. These are used to make an ideal mean image, which is compared to the real mean image to calculate the correction. Rather slow, can be useful for weak contrast)

half_acq.py [-h] [-i INTERACTIVE] [-a ACTIVATE] [-p PAD] scanname

Manage half acquisition / 360 degree scan reconstruction

(Inside tomodata, this is called automatically if you use "guess" to set the rotation axis.)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

                    Interactive mode [False]/True

  -a ACTIVATE, --activate ACTIVATE

                    Activate or disactivate an existing correction [True]/False

  -p PAD, --pad PAD   Padding to reconstruction size [default Auto]

launch_reconstruction.py [-h] [-i INTERACTIVE] [-b BLOCKSIZE] [-r ROI] [-t TIMEOUT] scanname

Launch reconstruction of volume with current parameters

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

                    Interactive mode [False]/True

  -b BLOCKSIZE, --blocksize BLOCKSIZE

                    Max blocksize in GB for 32bit .vol

  -r ROI, --roi ROI   Use ROI defined in par file True/[False]

  -t TIMEOUT, --timeout TIMEOUT

                    kill stuck pyhst job after N seconds

live_preview.py

Currently inside tomodata only.

(This watches a nominated spool directory. If new data arrives, it is reconstructed according to a protocol, which can apply rotation axis, paganin, etc. It always reconstructs the latest data, so if the scans arrive very fast it will skip older scans. It displays the last 6 reconstructions)

movement_correction.py [-h] [-i INTERACTIVE] [-f FILT] [-o OFF] [-l LINEAR] [-m MOVCOR] scanname

Tomography movement correction tool

(If there are calib images taken after the scan, will use these. Otherwise, will use the 0 and 180 degree images for a 180 degree scan, or the 0/90/180/270/360 images for a 360 degree scan. For 360 degrees it tries to find a linear rigid body movement of the sample.)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

Interactive mode [False]/True

-f FILT, --filt FILT high-pass filter length (slow!) [0]

-o OFF, --off OFF   Force off movement correction [False]/True

-l LINEAR, --linear LINEAR

Force linear 0-180 movement correction [False]/True

-m MOVCOR, --movcor MOVCOR

Movement correction file

Mercedes_movement_correction.py

Currently inside tomodata only.

(This is Wolfgang Ludwig's magic Mercedes correction, with some improvements. You select points in the reconstructed slice that you think are "point-like". The algorithm derives a movement correction to make the point-like.)

nonconstant_rings.py [-h] [-i INTERACTIVE] [-a ACTIVATE] [-n NSTEPS] [-c NCORES] [-p PIXELMASK] [-x FILTX] [-z FILTZ] scanname

Make, activate or deactivate double flatfield ring correction for non constant rings

(This is the same principle as double_ff, but instead of one correction for the whole scan it is broken up into angular steps. This means that if you have a rectangular section sample and the rings varying with angle, you can improve the correction. Creates new, corrected projection images which are then used by PyHST)

optional arguments:

 -h, --help   show this help message and exit

 -i INTERACTIVE, --interactive INTERACTIVE

Interactive mode [False]/True

-a ACTIVATE, --activate ACTIVATE

Activate (or disactivate) an existing correction [True]/False

-n NSTEPS, --nsteps NSTEPS

Number of steps in angle

-c NCORES, --ncores NCORES

Number of cores for multiprocess

-p PIXELMASK, --pixelmask PIXELMASK

Threshold for bad pixels (0=all pixels corrected)

-x FILTX, --filtx FILTX

Filter size (x, hor) for correction

-z FILTZ, --filtz FILTZ

Filter size (z, ver) for correction

paganin.py [-h] [-i INTERACTIVE] [-m MANUAL] [--pus PUS] [--puc PUC] [-o OFF] scanname

Find/change rotation axis in tomography data

optional arguments:

 -h, --help   show this help message and exit

 -i INTERACTIVE, --interactive INTERACTIVE

Interactive mode [False]/True

-m MANUAL, --manual MANUAL

        Specify Paganin length in pixels [25]

--pus PUS   Specify Paganin unsharp length in pixels [2.0]

--puc PUC   Specify Paganin unsharp coefficent [0.5]

-o OFF, --off OFF   Force off Pagainin filter [False]/True

preprocess_all.py [-h] [-i INTERACTIVE] [-a ACC] [-f {hdf5,edf}] [-b BIN BIN BIN] [-d SPOOLDIR] [--fast FAST] scanname

Tomography data preprocessing tool for PyHST

(This is behind option "s". Reads nxs or 32bit edf, writes 16bit edf for PyHST)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

        Interactive mode [False]/True

  -a ACC, --acc ACC   Accumulation factor for 32 to 16 bit conversion (auto = -1) [-1]

  -f {hdf5,edf}, --format {hdf5,edf}

        Data format [hdf5]/edf

  -b BIN BIN BIN, --bin BIN BIN BIN

        Bin projections [x y z]

  -d SPOOLDIR, --spooldir SPOOLDIR

        Where to look for the raw data

  --fast FAST   Fast (one sino, multiframe mode) [False]/True

preprocess_dimax.py [-h] [-i INTERACTIVE] [-a ACC] [-f {hdf5,edf}] [-b BIN BIN BIN] [-d SPOOLDIR] [--fast FAST] scanname

Tomography data preprocessing tool for PyHST

(Unpacks multi tif files from the ring buffer and camware of the Dimax into a number of tomos with the right number of projections)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

        Interactive mode [False]/True

 -b False, --bin False

        Bin projections 2x2

  -d SPOOLDIR, --spooldir SPOOLDIR

        Where to look for the raw data

preprocess_fast.py [-h] [-d DIR] [-s STEP] scanname

Preprocessing for a fast tomo sequence

(If you use synchroSnap etc in Tomo, and save a fast series of nxs files)

optional arguments:

  -h, --help   show this help message and exit

  -d DIR, --dir DIR   the spool directory

-s STEP, --step STEP   which step to preprocess

preprocess_spiral.py

Currently inside tomodata only.

(This treats a "tomo_spiral" acquisition. This is really a series of overlapping scans in the vertical direction. This function combines the projections using the nominal offset between scans without performing any image correlation. Works with the tomo_spiral function in SPyC)

recad_multi_memmap.py [-h] [-a LIMITLOW] [-z LIMITHIGH] [-f FORMAT] [-s SUFFIX] [-n NCORES] [-r REMOVE] [-i INTERACTIVE] scanname

Launch recad (32 -> 8 or 16 bit) of reconstructed volumes

(Uses a memory map to avoid having to read the whole 32bit volume into memory – a bit slower but no limit on volume size that I've hit yet)

optional arguments:

 -h, --help   show this help message and exit

 -a LIMITLOW, --limitlow LIMITLOW

                recad limit low

 -z LIMITHIGH, --limithigh LIMITHIGH

                recad limit high

 -f FORMAT, --format FORMAT

                convert to 8bit or 16bit [8bit]

 -s SUFFIX, --suffix SUFFIX

                suffix on .vol filenames _pag/[none]

 -n NCORES, --ncores NCORES

                multiprocess with how many cores [8]

 -r REMOVE, --remove REMOVE

                remove the .vol after recad [False]/True

 -i INTERACTIVE, --interactive INTERACTIVE

                Interactive mode [False]/True

reconstruct_all.py [-h] [-x REDO] [-r ROI] [-i INTERACTIVE]

Reconstruct all scans for an experiment

(I think I have always used this via tomodata. This probably needs a bit more separate documentation. The principle is as follows:

- *Decide if you need to preprocess data or not.*
- *Decide if you want to repeat reconstructions that have already been done (for example if you change parameters, or want to be sure that the same parameters are used everywhere)*
- *Decide if you want to treat spiral scans as separate scans, other where you want to combine the projections with preprocess_spiral.*
- *You can then select a subset of scans using a regular expression matching (i.e. sampleA_* will find sampleA_001, sampleA_002, etc).*
- *You can save and load lists of scans, which means you can select all the sample_*, but then edit the list to remove sampleA_test. It will save reconstruction_list.txt and preprocess_list.txt. You can rename these if you want.*
- *You can load a list of instructions (see later in this document).*

It is not super intuitive, and sometimes a bit awkward, but it can be very useful.)

optional arguments:

 -h, --help   show this help message and exit

 -x REDO, --redo REDO Reconstruct even if a volume exists

-r ROI, --roi ROI   Use ROI defined in par file True/[False]

-i INTERACTIVE, --interactive INTERACTIVE

> Interactive mode [False]/True

reconstruct_and_view.py [-h] [-i INTERACTIVE] [-s SLICE] [-t TIMEOUT] scanname

Reconstruct one slice and display the result

optional arguments:

-h, --help   show this help message and exit

-i INTERACTIVE, --interactive INTERACTIVE

> Interactive mode [False]/True

-s SLICE, --slice SLICE

> Slice to reconstruct [centre]

-t TIMEOUT, --timeout TIMEOUT

> kill stuck pyhst job after N seconds

remove_spikes.py [-h] [-n NCORES] [-k KEEP_ORIGINALS] [-i INTERACTIVE] scanname

Remove spikes with a 3 projection stackwise moving median filter

(Filters projections, creates corrected projections which are used by PyHST – inspired by Maxime's function that did the same thing. Good for high energies when the camera shielding is not effective enough)

optional arguments:

-h, --help   show this help message and exit

-n NCORES, --ncores NCORES

> Number of cores to use [16]

-k KEEP_ORIGINALS, --keep_originals KEEP_ORIGINALS

> Keep original images False/[True]

-i INTERACTIVE, --interactive INTERACTIVE

> Interactive mode [False]/True

roi.py [-h] [-i INTERACTIVE] [-r ROI ROI ROI ROI ROI ROI] [-x RESET] [-g GUI] scanname

Set the reconstruction ROI for a tomo scan

optional arguments:

-h, --help   show this help message and exit

-i INTERACTIVE, --interactive INTERACTIVE

> Interactive mode [False]/True

-r ROI ROI ROI ROI ROI ROI, --roi ROI ROI ROI ROI ROI ROI

> roi to reconstruct [x1, y1, z1, x2, y2, z2]

-x RESET, --reset RESET

> Reset roi [False]

-g GUI, --gui GUI   Use GUI selection of roi [False]

rotation_axis.py [-h] [-i INTERACTIVE] [-m MANUAL] [-f FILTER] [-g GUESS] scanname

Find/change rotation axis in tomography data

(Filter option is currently disactived, but could be useful sometimes maybe?)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

                    Interactive mode [False]/True

  -m MANUAL, --manual MANUAL

                    Specify rotation axis position

  -f FILTER, --filter FILTER

                    High pass filter length

  -g GUESS, --guess GUESS

                    Guess rotation axis position from motor positions

rotation_axis_by_reconstruction.py [-h] [-i INTERACTIVE] [-m MODE] [-n SLICENDX] [-j JUST_RUN] [-r READ] [-t TIMEOUT] scanname

Find rotation axis by reconstruction

(This works around the fact that one slice in PyHST has a ~20 second overhead. Instead of reconstructing N slices with different rotation axes, it builds an dataset in which the projections correspond to one line of the dataset, but shifted to shift the rotation axis. One reconstruction does 40 different rotation axes at once, and then we read the volume generated.)

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

                    Interactive mode [False]/True

  -m MODE, --mode MODE mode to optimise [std]/edges

  -n SLICENDX, --slicendx SLICENDX

                    slice to use

  -j JUST_RUN, --just_run JUST_RUN

                    Just run the reconstruction, dont change anything [False]/True

  -r READ, --read READ Just read the current reconstruction, dont reconstruct [False]/True

  -t TIMEOUT, --timeout TIMEOUT

                    timeout for PyHST in seconds [0]

select_name_only.py

Currently inside tomodata only.

     (This just selects a dataset from the local reconstruction directory)

utopec.py [-h] [-i INTERACTIVE] scanname

Replace partially obscured projections by darks

optional arguments:

  -h, --help   show this help message and exit

  -i INTERACTIVE, --interactive INTERACTIVE

Interactive mode [False]/True

view_only.py [-h] [-u UNIT] [-i INTERACTIVE] scanname

Display the current reconstructed slice

(Effectively what happens when you use option "n", or toggle the units)

optional arguments:

  -h, --help   show this help message and exit

  -u UNIT, --unit UNIT Unit for displaying images [mm]/pixel

  -i INTERACTIVE, --interactive INTERACTIVE

                  Interactive mode [False]/True

zero_clip.py [-h] [-v VALUE] [-i INTERACTIVE] scanname

Set zero clip value for a reconstruction

optional arguments:

  -h, --help   show this help message and exit

  -v VALUE, --value VALUE

                  Specify zero clip value

  -i INTERACTIVE, --interactive INTERACTIVE

                  Interactive mode [False]/True

Helper functions and things

In the ~/Python folder are some functions which are either not used in tomodata, or which are sub-functions that are not visible to the user.

call_pyhst.py

Helper function to call PyHST in interactive or batch mode, specific to the local installation.

check_reconstructions.py

Can be used in ipython to check that all volumes (.vol and/or .raw) are well reconstructed, with no problem to read and no blocks of all zero values.

fitting.py

Python functions for fitting Gaussian peaks profiles, etc.

load_beamline.py

Internal function that loads values from the BEAMLINE_PARAMETERS.par file.

maxime_tifffile.py

Maxime's copy of tifffile for reading and writing tiffs.

nslices.py

Set the NSLICESATONCE value in the par file. Needed for very large images where the default 300 causes the GPUs to run out of memory.

par_tools.py

Tools for reading, modifying, and writing par files. Reads pars into an ordered dictionary structure. Used everywhere.

stitch_spiral.py

If you have a spiral scan (really a series of overlapping scans in z) this will stitch them together using volume correlation (in x,y,z) to align them. At low resolutions, it is faster and simpler to stitch the projections together naïvely (without correlation) using preprocess_spiral.

total_variation.py

Setup the par file for total variation method implemented in PyHST. Probably needs work.

Instructions files for scripting or batch processing

In tomodata, the option "A" (reconstructAll.py) allows you to batch process a series of scans. The option "live" (live_preview.py) allows to follow a acquisition in progress. In both cases, you may need to use a list of instructions. I usually call this "protocol.txt" or similar. An example is given here:
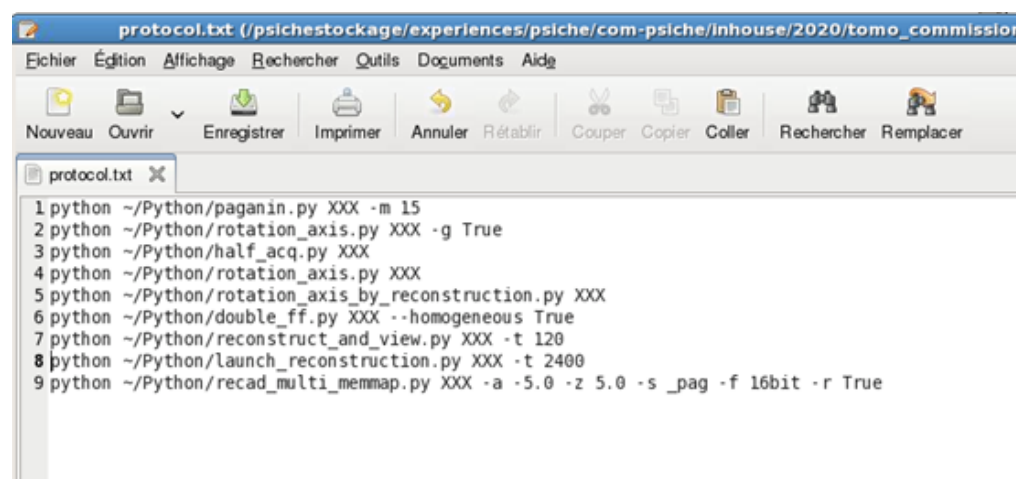
The file consists of the functions to be applied, as if they were called from the command line, in the working directory. The scanname is replaced by "XXX".

In live_preview, the slice will be reconstructed automatically, so you do not need to put reconstruct_and_view in the protocol. In reconstruct_all, if you load instructions, then the instructions should contain launch_reconstruction or reconstruct_and_view. If you don't load instructions, it will simply call launch_reconstruction on each scan.

(Added by T. Weitkamp on 17 February 2021:) Below is another example of a "protocol.txt" file with batch-processing instructions, taken from an experiment that used offset scans (="half acquisition"):

Example "protocol.txt" for offset scan

```
python ~/Python/pentezone.py -v 200
python ~/Python/rotation_axis.py XXX -g True
python ~/Python/rotation_axis.py XXX
python ~/Python/half_acq.py XXX
python ~/Python/double_ff.py XXX -x 9 -z 9 -n 1
python ~/Python/paganin.py XXX -m 50
python ~/Python/reconstruct_and_view.py XXX
python ~/Python/launch_reconstruction.py XXX
```

See also

- PyHST documentation at ESRF: http://ftp.esrf.fr/scisoft/PYHST2/

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