Enhanced and Flexible Software Tools for X-ray Computed Tomography at the Italian Synchrotron Radiation Facility Elettra

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Abstract. X-ray computed tomography (CT) experiments performed at synchrotron radiation facilities require adequate computing and storage resources due to the large amount of acquired and reconstructed data produced. To satisfy the heterogeneous needs of beamline users, flexible solutions are also required. Moreover, the growing demand of quantitative image analysis impose an easy integration between the CT reconstruction process and the subsequent feature extraction step. This paper presents some of the software solutions adopted by the SYRMEP beamline of the Italian synchrotron radiation facility Elettra. By using the enhanced version of the reconstruction software here presented as well as data reduction and data analysis tools, beamline users can easily implement an integrated and comprehensive approach to the digital image processing and image analysis required by a tomography-oriented scientific workflow.

Keywords: computed tomography, image reconstruction, image processing, image analysis, computing workflow

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1. Introduction

Within the whole scientific workflow that starts from a beamtime request and leads to one or more scientific publications, an effective X-ray computed tomography (CT) experiment at a synchrotron radiation facility requires more than the optimization of the raw data acquisition and reconstruction processes. There are steps that have to be performed at user's home institution before the data collection at the facility such as e.g. sample preparation. More interestingly, there is also a growing demand of data reduction and data analysis tools in order to support the qualitative evaluation of the images with quantitative measurements of significant parameters derived from the reconstructed data.

The visualization of reconstructed data as well as its reduction and analysis can be performed either at user's home institution or during the beamtime, if proper software is offered by the facility. When collecting tomographic data one highly desirable goal is to reconstruct and visualize the data in less time than it takes to collect. In that case it is then possible to examine the previously acquired dataset even before the next acquisition is complete, allowing rapid feedback on data quality and experimental conditions. If also a preliminary data reduction and data analysis could be performed, a global optimization of the whole tomographic-based scientific workflow would be possible leading to more effective experiments and better user's satisfaction.

Although typically the data is reconstructed at the facility during the beamtime, there are several cases when it would also be very useful for the users to be able to reconstruct the data at their home institutions. Users aim to push the frontiers of their studies towards new domains which require the best image quality achievable so they may need to optimize one or more steps of the reconstruction process with a fine tuning of the reconstruction parameters. Moreover, they may want to consider customized intermediate steps with state-of-the-art software tools available at their home institutions or even by taking advantage of third party tools and collaborators. Therefore it would be very useful to be able to reconstruct large datasets (larger than the available memory) in reasonable time on computers that users are likely to have available locally [15] and/or to offer remote reconstruction and analysis tools to be used from their home institution [8]. In order to reconstruct and analyze the produced data, adequate solutions must be adopted to fit the limits of the available computing power and storage resources without sacrificing image quality. The answer to these requirements is a continuous development of advanced computer science approaches as well as refined digital image processing for CT.

It is here presented the data reconstruction solution adopted by the SYRMEP [16] beamline of the Italian synchrotron radiation facility (Elettra - Sincrotrone Trieste S.C.p.A.) where nearly-parallel beam X-ray CT experiments are routinely performed. This software solution is named *SYRMEP Tomo Project* and, when combined with the data reduction and data analysis tool *Pore3D* [3], it offers an integrated and comprehensive approach to the image processing and image analysis required by a tomography-oriented scientific workflow. These tools are an effective and flexible solution suitable for the SYRMEP scenario where the subtle line between what can be done during a beamtime and what can be done at user's home institution is continuously shifted to satisfy the specific requirements of different users.

2. Software description and features

The *SYRMEP Tomo Project* (STP) is an in-house software suite composed by newly developed code as well as external libraries. Originally developed to support absorption and edge-enhanced phase-contrast experiments by offering only the essential pre-processing and the filtered back projection (FBP) reconstruction algorithm, it has recently been re-designed in order to effectively integrate single distance propagation-based phase-contrast experiments [1] where phase retrieval [11] is required. Moreover, additional reconstruction algorithms better suited for low-dose or fast CT, where a reduced number of noisy projections is collected, are now available. More attention to the computational performances has also been paid by re-writing portions of the original code with parallel and/or GPU implementations. The STP has a graphical user interface and it is conceived to offer flexibility for the SYRMEP users in terms of an easy switch between a local (at the facility) and remote (from the home institution) access. A few interesting peculiarities of this software suite are hereafter presented.

2.1. Pre-reconstruction Image Processing

Tomographic reconstruction belongs to the class of computational problems which are often referred to as “embarrassingly parallel” [5]. Essentially, such problems can be decomposed into smaller independent units and computed in parallel. In fact, before considering instruction-level parallelism, a very simple way to decompose the volume reconstruction problem exists when dealing with parallel beam data acquired with a bi-dimensional (2D) detector. In this case a (non-parallel) implementation of a tomographic reconstruction algorithm can be executed on each sinogram image independently. However, the digital image processing required to produce a three-dimensional (3D) image from the acquired 2D projections does not consist in the mere application of a reconstruction algorithm, such as FBP or an algebraic method [7]. A pipeline of several pre-reconstruction steps is necessary, such as e.g. flat fielding, hot/dark pixel correction, artifacts removal and gray level calibration. All these steps affect the computational time of the global reconstruction process in a non-negligible way. More significantly, their application does not guarantee that a global independent and parallel execution of 2D image processing algorithms ”from acquired to reconstructed” can be performed. Barriers and synchronization methods are required after each intermediate step.

A basic distinction can be performed between projection-order and sinogram-order pre-processing. While some of the pre-reconstruction steps are traditionally faced by processing each 2D projection (e.g. phase retrieval), other steps are usually effectively handled by processing each sinogram (e.g. ring removal [2]). Moreover, the order of the steps in the pre-processing pipeline might significantly affect the image quality. A strategy for e.g. dark/hot pixel correction might prefer to process raw data projections while another strategy performs better after flat fielding correction. A ring artifacts compensation technique can in principle be applied before or after (or also two times, i.e. before and after) the phase retrieval step. Therefore, a frequent switch between the projection-perspective and the sinogram-perspective of the dataset is necessary in a flexible pre-processing pipeline. This frequent perspective switch requires intermediate I/O since the imaged data to process is usually larger than the available memory.

2.2. Tomo Data Format

Due to the sequential nature of the acquisition process and the limitations of 32-bits file systems, in the past decades a sequence of 2D image files (usually a TIFF file for each acquired projection as well as flat/dark images) was the most common way to store in a file system a synchrotron radiation CT raw dataset. Although there is still no agreement in the CT community for a unique file format (both for synchrotron and desktop facilities), the general trend is to move towards a volume file format able to effectively handle large datasets. Thanks also to the advances of file systems, the HDF5 technology[1] seems to be suitable for these purposes [4].

The STP software exploits a custom HDF5-based file format named TDF (Tomo Data Format) that follows the DataExchange initiative [4]. Although detectors vendors are now starting to support HDF5 in their device driver, the vast majority of the detectors used at SYRMEP still outputs a TIFF file for each acquired projection. A conversion process from the sequence of TIFF files to TDF is therefore necessary. Although this conversion can be done after the whole acquisition is complete, a better strategy consists in performing the conversion during the acquisition process. A software service listens to the projection files produced by the detector control software and it simultaneously transfers the data to a network storage with a suitable file system (or to the hard drive of a dedicated reconstruction machine) while filling the TDF container. In this way the computational time of the whole CT workflow is not affected by this file format issue. Moreover, a TDF file does not contain only the raw data but it can store useful experimental metadata such as, for instance, acquisition energy, sample-to-detector distance and detector pixel size. These details are also necessary for some pre-processing algorithm (e.g. phase retrieval). The TDF container can also include details about the computational steps applied on it (data provenance), which is another key advantage. Since HDF5-based files are containers of multiple information, this allows for a much lower number of files per dataset.

While the hierarchical data organization of a HDF5 file allows an easy switch between projection- and sinogram- perspectives, the I/O performances are however different in the two domains since bytes are contiguously organized within the file for only one of the two perspectives. Although the situation can be easily switched by toggling a flag during the conversion process, the default setting in the STP software privileges fast I/O in the sinogram domain. The reason for this is that an essential set of image processing steps includes at least the flat fielding and this can be easily faced in the sinogram domain. Moreover, it is worthy to remind that all the parallel beam CT reconstruction algorithms require a sinogram as input. Also, during a beamtime users are usually interested in a very fast reconstruction of just one slice image in order to have a rapid feedback on image quality and the experimental protocol as soon as the acquisition is complete. Although it is difficult to propose a standard reconstruction workflow and flexibility is a key paradigm of the STP, sinogram domain steps are usually more frequent in a CT pipeline and therefore a data organization that privileges I/O in the sinogram perspective is more desirable.

As aforementioned, if all the pre-processing steps occur in the sinogram domain, an embarrassingly parallel solution that goes from the acquired raw data to the reconstructed images comes straightforward and there is no need of intermediate I/O. In this case there is no significant computational benefit of the adoption of a HDF5-based file format, provided that a conversion from the sequence of 2D projection files to a sequence of 2D sinogram files (in e.g. TIFF format) is performed during the acquisition process. If a 2D file format is requested for each reconstructed slice, a job submission of the global reconstruction process to a High Performance Cluster (HPC) is in general recommended for this scenario. However, while mixing sinogram- and projection-order image processing (in arbitrary order) there is the need to perform intermediate I/O due to the large amount of data to process. Without the adoption of a 3D format, a significant portion of the total processing time would be wasted in conversions from 2D projection files to 2D sinogram files with also the need of more storage occupation for intermediate data. Moreover, when mixing sinogram- and projection-order processing, the whole CT reconstruction problem is no

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[1] `http://www.hdfgroup.org`

more embarrassingly parallel since barrier mechanisms are required to synchronize after e.g. a sinogram-domain step before a projection-domain step and viceversa. This synchronization mechanism combined with the I/O of intermediate data could significantly slow down the global process. In this scenario, if the amount of data is relatively small, a solution on locally available hardware resources might perform faster than an execution on remote HPC resources where parallel I/O (Message Passing Interface - MPI with a parallel file system) to a 3D HDF5 file are also another issue to consider. The STP takes into account this aspect by facing the reconstruction problem either locally or on a HPC, depending on the amount of data and the selected pre-processing pipeline of the specific experiment.

2.3. Tomographic Reconstruction

The Filtered Back Projection is the most widely adopted algorithm in CT reconstruction workflows and it is generally recognized as the fastest way to produce adequate results when a sufficient number of projections is acquired. A complementary approach is based on algebraic reconstruction techniques. The advantages of the algebraic approach include improved insensitivity to noise and capability of reconstructing an optimal image in the case of incomplete data. Algebraic approaches are generally considered superior when a large set of projections is not available, when the projections are not distributed uniformly in angle, when the projections are sparse or missing at certain orientations and when metal artifacts require the exclusion of some portions of the projection data.

Algebraic methods for tomography reconstruction were widely disregarded in practical applications due to the substantial amount of inherent computational effort. However, the continuously growing computational power of today's standard computers has led to a rediscovery of these methods. These reconstruction methods might be interesting for users performing, for instance, experiments in which the radiation dose is a concern and therefore a limited number of projections is acquired. The re-designed STP aims at maintaining the state-of-the-art in this field by offering not only a single reconstruction algorithm (i.e. FBP) but also algebraic techniques. The *SYRMEP Tomo Project* is powered by ASTRA [13] and TomoPy [6]. It integrates also publicly available reconstruction libraries (see e.g. [14] and [9]) as well as custom developed algorithms.

Within the reconstruction process, a time consuming task is the determination of the pixel in the acquired images to be assumed as the rotation axis. Ideally, once the acquisition setup is established, the center of rotation should be known a priori and it could be adopted throughout the experimental session. However, it is often necessary to "tune" the center for each dataset, because of mechanical imperfections in vertical or horizontal translation stages, thermal drifts, etc. Moreover, if the tomography system is perfectly aligned then the rotation center should be the same for all slices in the sample. However, there may be a slight misalignment of the rotation axis and the columns of the CCD detector, such that there is a systematic change in the optimum rotation axis from the top to bottom of the sample. The STP offers automatic strategies for the determination of the center of rotation in order to speed-up this time consuming task.

3. Example of application

In order to show the benefits in terms of image quality when users can test different reconstruction algorithms and phase retrieval, this section presents a few results produced by the re-designed *SYRMEP Tomo Project*. Though there are significant computational differences in the considered algorithms and, more generally, in the whole reconstruction workflow, computational performances are not taken into account here.

3.1. Materials and Methods

A test object (hereafter also referred as phantom) with known composition was considered [10]. The phantom consists of a polyoxymethylene (CH_2OH) cylinder, 16 mm in diameter, in which six holes of 3 mm diameter have been drilled parallel to the cylinder axis. The holes were filled with water (H_2O), paraffin wax ($C_{25}H_{52}$), glycerol ($C_3H_8O_3$), glucose ($C_6H_{12}O_6$) 10g/50ml, glucose 23g/50ml, and one of them was left empty (see Figure 2).

The phantom was scanned at the SYRMEP beamline with the following experimental parameters: energy = 21 keV, sample-detector distance = 300 mm, water cooled 12 bit CCD camera (Photonic Science VHR, 4008×2672 pixels used in 2×2 binning mode resulting in pixel size = 9 μm) coupled to a Gadolinium Oxysulphide scintillator placed on a fiber optic taper. In this application, a value $\delta/\beta = 2178$ was adopted when applying Paganin's phase retrieval [12], where β is the imaginary part and δ the decrement from unity of the complex X-ray refractive index $n = 1 - \delta + i\beta$. This value $\delta/\beta = 2178$ was taken from a publicly available database[2] and it corresponds to the refractive index of the polyoxymethylene at 21 keV.

Before the actual reconstruction, the projections were flat-field corrected and normalized by considering the air windows on the left and right side of the image as a reference. Then a ring removal filter [2] was applied in order to better compensate the detector inhomogeneities. When considered, phase retrieval was performed at this stage. Then, after the application of a reconstruction algorithm, images were calibrated in order to have a coherent gray scale for all of them. The calibration was performed by selecting the mean gray level of two meaningful and homogeneous areas in the image. A linear rescaling was then applied to each image. A chart of the pipeline used to produce the images presented in the subsequent figures is reported in figure 1.

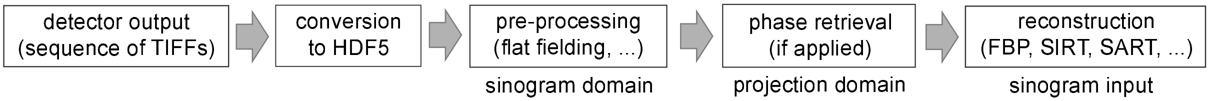

Figure 1. Chart of the image processing pipeline used in the considered experimental application to produce a reconstructed image starting from the detector output.

In addition to the FBP, the considered reconstruction algorithms are: Simultaneous Iterative Reconstruction Technique (SIRT), Simultaneous Algebraic Reconstruction Technique (SART), Conjugate Gradient Least Squares (CGLS) [13], Equally Sloped Tomography (EST) [9] and Minimum Residual FBP (MR-FBP) [14]. The same number of projections was considered for all the algorithms but the non-linearly spaced angles that better approximate the requirements of the equally sloped tomography approach were adopted for the EST reconstruction.

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[2] `https://ts-imaging.net/Services/Simple/ICUtilXdata.aspx`

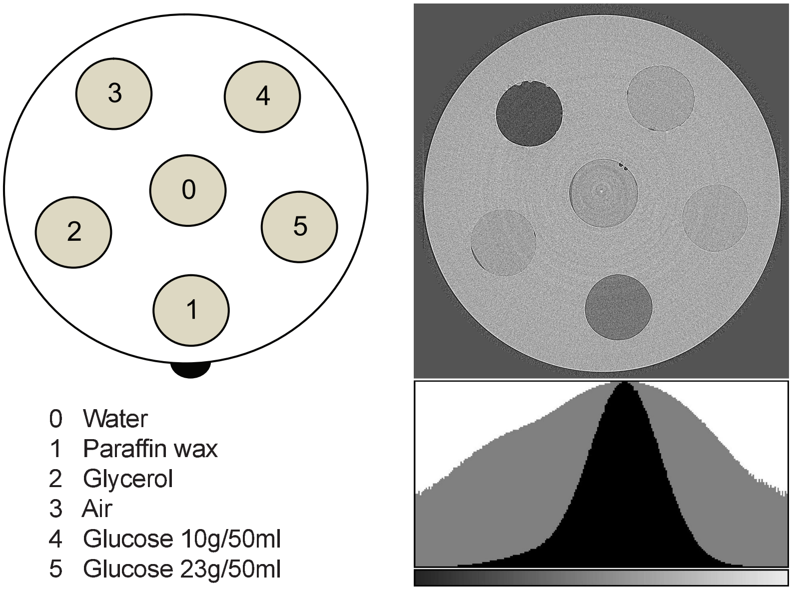


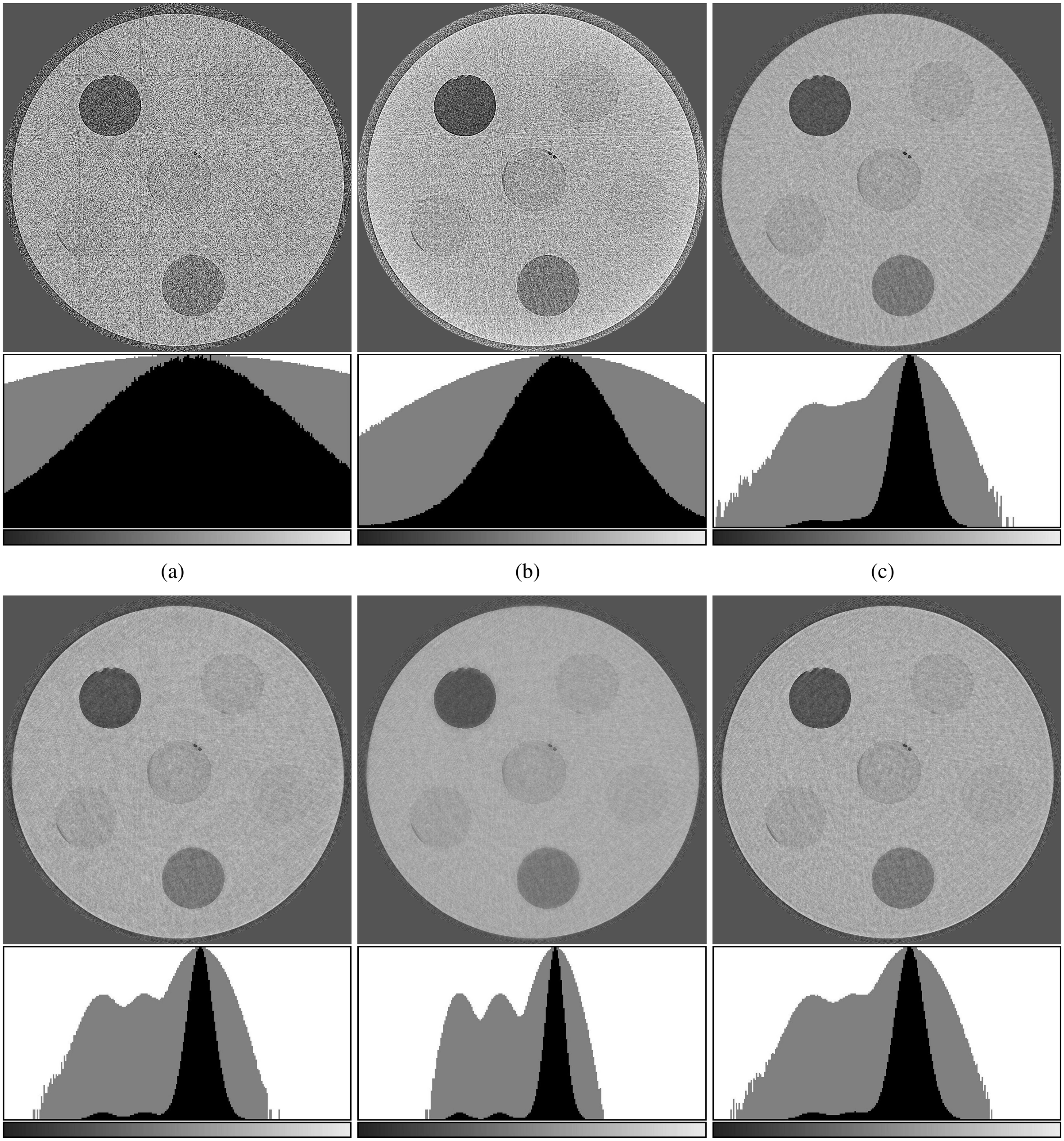
Figure 2. Sketch of the phantom considered in this application and edge-enhanced phase-contrast image reconstructed with FBP and 720 projections. Difficulties in image segmentation and further analysis arise due to the monomodal gray level histogram. [Linear scale gray level histogram in black and logarithmic scale in gray]

3.2. Results

Figure 2 reports the edge-enhanced phase-contrast image obtained by applying the FBP reconstruction algorithm (with Shepp-Logan filtering) after simple flat-fielding and ring removal when considering 720 projections. By observing the gray-level histogram it can be noticed that image segmentation and further analysis might be hampered due to the monomodal distribution of gray tones.

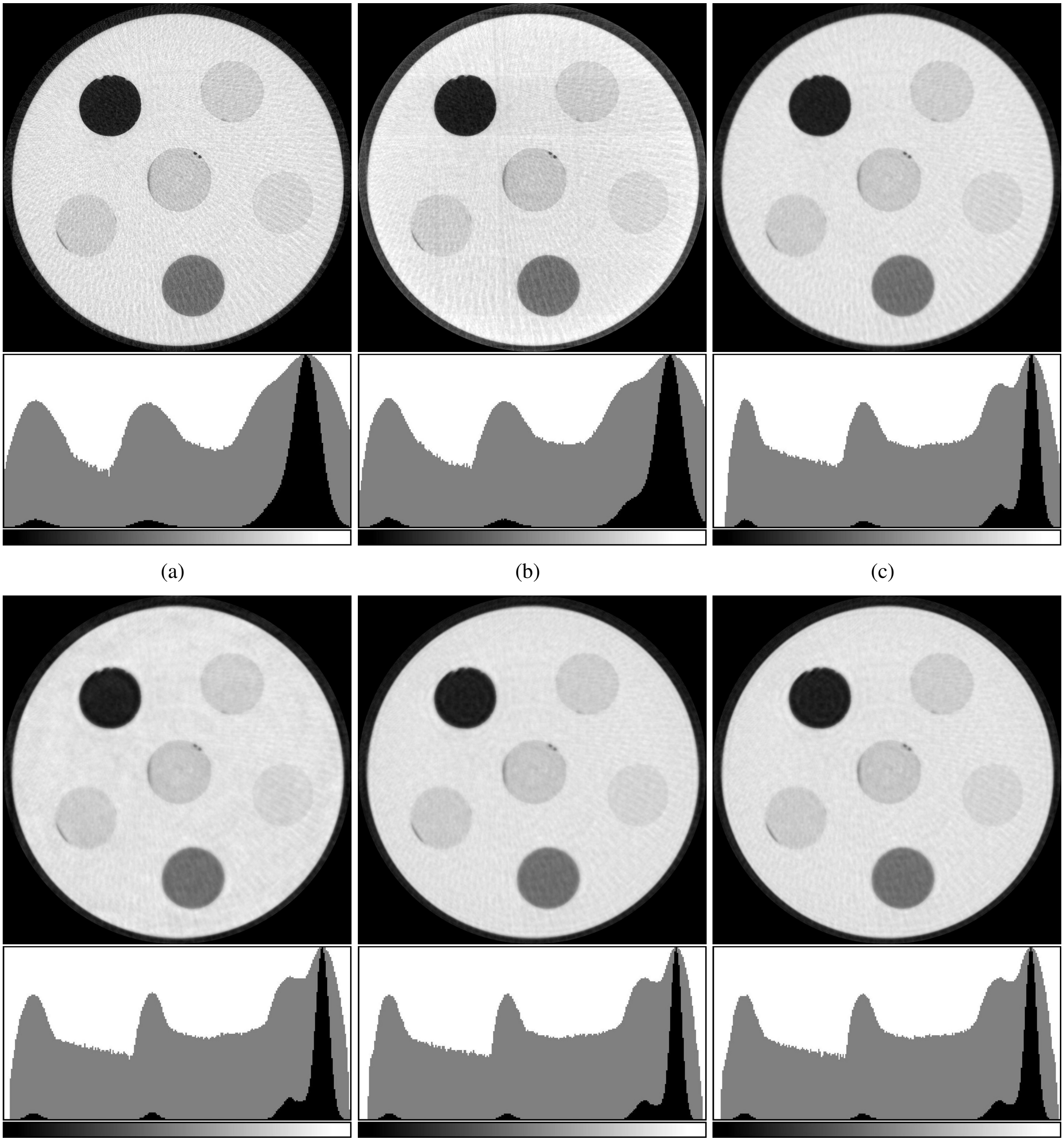
Figures 3 reports the output of different reconstruction algorithms after the application of the same pre-processing steps when considering 90 projections (meaning 1/8 of the acquisition time and radiation dose of the reference image). Figure 4 reports the results of the application of the same algorithms but with the addition of the intermediate phase retrieval step before the actual reconstruction. It can be noticed that while the most classical approach based on FBP without phase retrieval leads to a noisy image where the different holes in the object can barely be recognized, iterative algorithms combined with phase retrieval are able to reconstruct images having multi-modal histogram where the inclusions within the phantom can be more easily segmented. Interestingly, promising results are obtained with the SIRT algorithm also without the application of phase retrieval. However in the images reconstructed after phase retrieval the phase-contrast fringes at the edges of the drilled holes in the phantom are correctly integrated and a better separation of the peaks in the image histogram is noticeable.

Several applications can greatly benefit from such an enhanced and flexible reconstruction workflow where phase retrieval and iterative algorithms can be used. When the whole image processing pipeline can be applied in a reasonable amount of time, CT acquisitions with a reduced number of projections are possible leading to a minimization of the radiation damage, faster experiments or, simply, more samples per beamtime.



(a)
(b)
(c)
(d)
(e)
(f)

Figure 3. Reconstructed images when considering only 90 projections according to the following algorithms: a) FBP; b) EST; c) MR-FBP; d) SART; e) SIRT; f) CGLS. The related gray level histogram is reported below each image (the same gray level window was used for all the images). [Linear scale gray level histogram in black and logarithmic scale in gray]



(a) (b) (c)

(d) (e) (f)

Figure 4. Reconstructed images after the application of phase retrieval when considering only 90 projections according to the following algorithms: a) FBP; b) EST; c) MR-FBP; d) SART; e) SIRT; f) CGLS. The related gray level histogram is reported below each image (the same gray level window was used for all the images). [Linear scale gray level histogram in black and logarithmic scale in gray]

4. Conclusion

The *SYRMEP Tomo Project* suite was presented here as a flexible software solution conceived for the scenario of the SYRMEP beamline at Elettra where both remote and locally available software tools are required in order to satisfy the specific requirements of the users. It implements different reconstruction techniques and several options for an effective image pre-processing including also single-distance phase retrieval. To better appreciate the benefits of this, especially when fast and/or low-dose experiments have to be performed, the manuscript presents a comparison of different reconstruction algorithms combined with phase retrieval. The advantages of a HDF5-based file format named TDF (Tomo Data Format) were also presented and it was shown why this file format positively affects the reconstruction workflow both from the computational and flexibility points of view.

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