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A Python-based package for X-ray phase contrast imaging data analysis and CT reconstruction: first developments

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ABSTRACT: X-ray imaging has improved significantly as a high-resolution and non-invasive probe to detect the internal structures of samples in different fields. While the conventional absorption contrast method is particularly beneficial for characterising medium-density samples (but not for low-Z materials), Phase Contrast X-ray imaging is an effective technique for detecting low contrast details in weakly absorbing samples. As such, it has great potential in many fields of application, delivering high-quality information on micro-structural features. X-ray Grating Interferometry is one of the techniques vastly adopted at both synchrotron facilities and laboratories for phase contrast analysis, where the diffraction patterns generated by gratings are used to extract phase information. In this paper, a Python-based package for signals extraction (absorption, differential phase and dark field) and computed tomography reconstruction is illustrated; the code is developed in the framework of the PRIN2022 PITCH Italian project, based on a Metaljet X-ray source in a laboratory setup installed at the University of Torino, and focused on the analysis of Cultural Heritage materials. This package can be used through preset Jupyter Notebooks for the different tasks; also, a user-friendly GUI is in preparation.

KEYWORDS: Computerized Tomography (CT) and Computed Radiography (CR); Image processing; Inspection with x-rays; Interferometry

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1 Introduction

In recent decades, X-ray imaging has improved significantly as a high-resolution and non-invasive tool for radiography and tomography, solving the major challenge of detecting the internal structures of samples in different applications. The different types of interaction mechanisms of X-rays with matter (described by the complex refractive index $n = 1 - \delta + i\beta$) provide specific and complementary information on the characteristics of the sample. Conventional X-ray imaging maps the attenuation coefficient of materials, which depends mainly on the atomic number (Z) and is described by the imaginary part of the refractive index (β), poorly sensitive to weakly absorbing materials. Instead, phase contrast (PC) X-ray imaging, which is linked to the real part of the complex refractive index (δ), allows visualising soft materials, relying on the phase shift or the refraction of X-rays caused by the object [1]. This method is based on the observation of the interference pattern between diffracted and non-diffracted waves introduced by a sample placed on the wave path. PC imaging has great potential in medical, material science and cultural heritage applications, since it can provide high-quality information on micro-structural characteristics [2, 3]. This method has already been deployed in synchrotron facilities thanks to extremely coherent X-ray beam [4, 5]. Among PC methodologies, X-ray Grating Interferometry (GI), which provides differential phase and scattering (dark-field) images in addition to the standard absorption-based image, enables the assembly of systems implementable in a laboratory setting with the use of diffraction gratings [6, 7]. This scenario opens interesting opportunities in different fields of research, including cultural heritage. In the context of the PITCH Italian project (funded by MUR, PRIN2022 program), a GI laboratory setup based on a Metaljet X-ray source has been developed at the University of Torino, focused on the analysis of Cultural Heritage materials [8]. The project, aimed at different goals, involves also the University of Milano-Bicocca, the Istituto Nazionale di Fisica Nucleare (INFN) and the Centro per Conservazione ed il Restauro dei Beni Culturali (CCR) “La Venaria Reale”. A very important step concerns the in-house development of software for data processing, allowing a full control and customisation of the algorithms for CT reconstruction, which are less developed in the context of PC-GI imaging with respect to traditional absorption imaging. In this framework, Python-based packages for extracting specific signals (absorption, differential phase, and dark field) and reconstructing computed tomography (CT) have been assembled and will be described in the following sections.

2 Materials and methods

2.1 Laboratory set-up

The X-ray GI system of the PITCH project (figure 1) was implemented using a liquid-metal-jet source provided by Excillum (Metaljet D2+) [9]. This new generation of X-ray sources features a liquid-jet anode made of an In-Ga-Sn alloy with energy peaks at 9.3 and 24.2 keV. It has a focal spot size in the 5–30 μm range, voltage, current and power up to 160 kV, 4.3 mA and 250 W respectively, and operates in cone beam configuration. The increased photon flux of this metal-jet source, if compared to the conventional microfocus X-ray tubes ($\sim \times 10$), improves GI performance and reduces exposure time, particularly for tomographic investigation. The system is equipped with three periodic gratings (Talbot-Lau system): i) a silicon source grating (G0), in front of the tube's exit window, ii) a gold phase grating (G1), between the source and the sample, and iii) a silicon analyser (G2) in front of the detector. The system has a symmetric arrangement with the same period ($p = 5.25 \mu\text{m}$) for all gratings and is designed for an energy of 45 keV. The size, due to the 100 μm wafer micro-fabrication technology, is about $7 \times 7 \text{ cm}^2$, which constrains the system field of view (FoV). A precision rotatory stage on a dedicated mechanised platform and a flat panel CMOS detector with an $11 \times 14 \text{ cm}^2$ active area and 49.5 μm pixel size are used. The gratings and the detector are mounted on a linear stage platform which can translate the components along the beam direction. By doing this, distances between the different components can be adjusted to optimise the FoV size and magnification based on the samples being examined. Hexapods are also employed for grating alignment and data acquisition (phase stepping and "Moiré" methods [10]). Therefore, the G2 grating is equipped with a motorized goniometer for Moiré imaging. The X-ray source is fixed and placed on a granite optical bench; the entire system is mounted in a thermally controlled hutch. All the movement systems and data acquisition are controlled via an in-house developed LabView 2019 SP1 software.

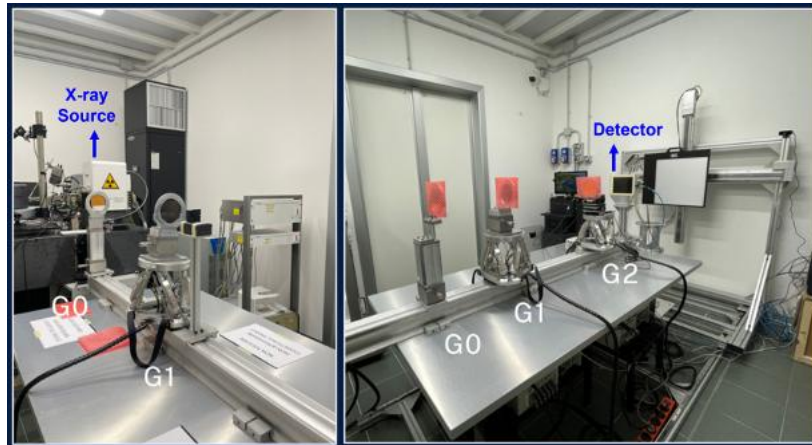


Figure 1. Laboratory GI setup of the University of Torino.

2.2 Data analysis tools

In the project context, a tool for GI data analysis was written in Python (v.3.11.7), as open-source, cross-platform, and human-readable programming language and was developed in Jupyter environment. Different notebooks were prepared for each step of data analysis; for each notebook, specific modules

with purpose-developed functions are used. The entire data analysis chain is represented in figure 2. The different modules exploit several Python libraries for scientific computing and image processing, i.e. NumPy, SciPy, Scikit-Image, OpenCV and Matplotlib. In particular, the CT reconstruction step is powered by the ASTRA Toolbox [11].

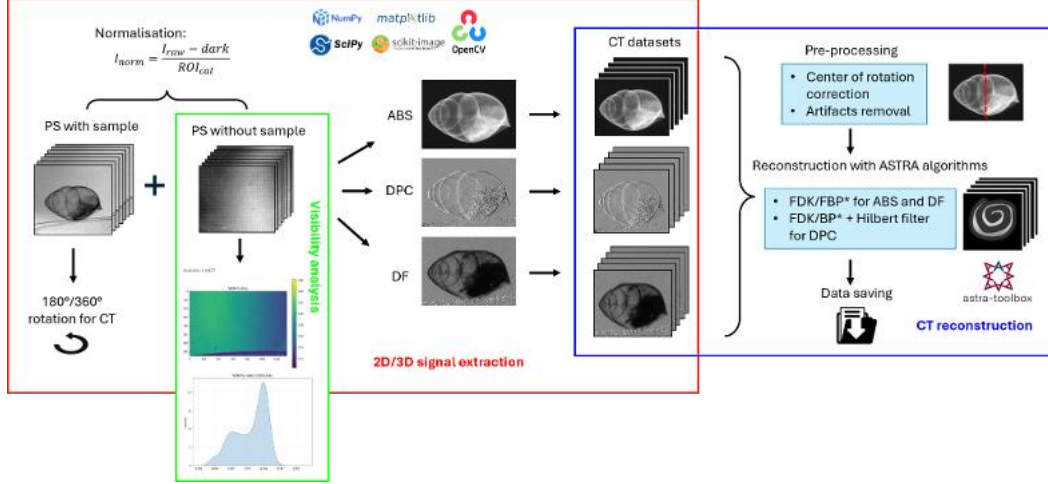


Figure 2. Schematic data analysis workflow: coloured boxes refer to different set up Jupyter notebooks (PS=phase stepping; ABS=absorption; DPC=differential phase contrast; DF=dark field).

The first task is represented by extracting the signals from the collected raw data. In this case, phase stepping (PS) is used as data acquisition method. The specific notebooks (one for 2D and another for 3D tomographic data) use custom implemented modules for reading, normalising, and extracting the three signals (`prepare_data`, `psc_sine`, `psc_fourier`). In addition, a further specific notebook has been developed for visibility analysis [10]. In the code snippet 1 are three examples of functions related to the cited modules, imported as `pd`, `ps` and `pf` respectively. TIFF files of the raw data (flat, sample and dark images) are loaded and converted into numpy arrays through a specific function that takes files paths and a pre-compiled .txt file containing metadata as input (`pd.image_prepare`). In this step, dark subtraction is also applied and a preview of the resulting flat and sample images can be visualised. A background normalisation is then applied by selecting a region of interest (ROI) corresponding to a background area not covered by the specimen (both for flat and sample, in the code it is called “calibration ROI”, see equation in figure 2). Even the area to be normalised has to be selected (named “big ROI”). These regions of interest can be specified in two different ways: drawing interactively a rectangular selection (`pd.select_bigroi_calroi`) or reading an ImageJ .roi file (`pd.get_coordinates_from_roi`); only then, normalisation functions can be used (`pd.normalization_from_draw` and `pd.normalization_from_coord` based on the method used for ROIs selection). These functions return a 3D array containing the stack of normalised sample and flat images. Subsequently, signals extraction can be performed with two different methods for 2D analysis, sine fitting and Fast Fourier Transform (FFT) [10]; only the latter is implemented for tomographic data. The sine fitting function allows estimating the parameters exploiting the entire selected ROI (`ps.sine_fitting_ROI`); these parameters can be in turn used as initial values for the final fit (e.g. `ps.sine_fitting_3D_rows`, both for flat and sample images, see figure 3). The resulting fit can be visualised both for the entire ROI and the single pixels. Instead,

function `pf.psc_fft` is used for the Fourier method. The three signals are then obtained using `ps.sine_fitting_result` and `pf.psc_fft_result` for sine and FFT respectively.

```
# DATA LOADING
flat, sample = pd.image_prepare( dark_path, flat_path, sample_path,
                                dark_name, n_step, bool_print=True)

# SINE FITTING
fit_3D_sample = ps.sine_fitting_3D_rows(sample_norm, n_step, out,
                                         est_a0=0.57, est_a1=0.04, est_phi=0.51, bool_print=True, bool_save=False)

# FFT
rec_flat, rec_sample = pf.psc_fft(flat_norm, sample_norm)
```

Code snippet 1. Function examples of modules *pd=prepare_data*, *ps=psc_sine*, *pf=psc_fourier*.

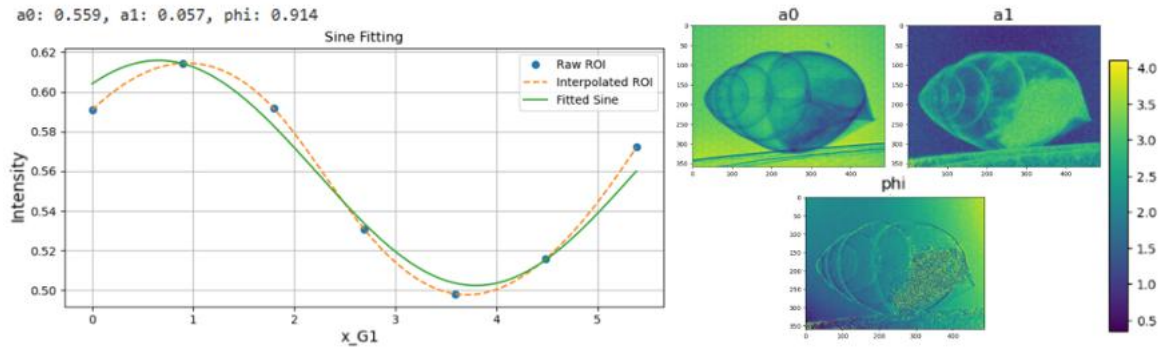


Figure 3. Example of sine fit with estimated parameters and graphical results. Values on the x-axis correspond to G1 grating positions (μm).

Once attenuation, differential phase and dark field images are obtained, the CT reconstruction pipeline can be performed through another specific pre-compiled notebook, which includes tools for centre of rotation correction, ring artifacts removal and volumes reconstruction. As already described above, a stack of projections is loaded as a 3D numpy array. Once geometric data (source-object-detector distances, angles, pixel size) have been specified, some functions for offset calculation (misalignment of the rotation axis with respect to the vertical axis of the detector) can be used. The automatic ones (`rec.find_cor_correlation` and `rec.find_cor_iqm`) can provide the offset estimate through three different methods (correlation for the former, entropy and sharpness as image quality metrics parameters for the latter [12, 13]). A manual function (`rec.find_cor_manual`) can be used to reconstruct a slice with a different centre of rotation (the offset range can be manually selected by the user), visualise the results and finally choose the optimal offset value for the subsequent correction. The offset calculation is currently performed on the central slice (corresponding to the central detector row), but a method for tilt angle correction and artifacts correction tools (e.g. ring artifacts correction with destriping filters) are under development [14]. The reconstruction routine includes all GPU-based algorithms for 3D beam geometry (in this case, cone beam geometry) implemented in the ASTRA toolbox (e.g., FDK_CUDA, see online documentation). This can be used to reconstruct absorption contrast and dark field volumes, also using associated

parameters such as filters or number of iterations. Differential phase contrast projections are instead previously filtered by using a modified filter kernel (base on Hilbert transform) [15], in such a way that the volume can be reconstructed through the BP3D_CUDA algorithm. The tool developed to perform a CT reconstruction is `rec.rec_volume(matrix, angles, pixel_size, SOD, ODD, offset, img_type, method, parameters)`, where *matrix* is the stack of projections, *angles* is a one-dimensional array containing the view angles in radians, *pixel_size* is the detector pixel dimension, *SOD* and *ODD* are the geometric distances, *offset* is specified for centre of rotation correction, *img_type* is a string to specify the projection type (absorption, dark field and differential phase) in order to enable the pre-filtering process for DPC, *method* indicates the algorithm to use and *parameters* relates to specific settings of the reconstruction algorithm (e.g. filters or number of iterations). Examples of reconstruction functions of absorption (abs) and differential phase contrast (dpc) CT can be found in code snippet 2. The reconstructed volume can be saved on the computer as a 32-bit .tiff image stack using a specific function (`rec.save_rec`).

```
# ABS PROJECTIONS
rec = rec.rec_volume(proj, angles, SOD, ODD, offset=0.5, img_type='abs',
                    method='FDK_CUDA', parameters='hamming')

# DPC PROJECTIONS
rec = rec.rec_volume(proj, angles, SOD, ODD, offset=0.5, img_type='dpc',
                    method='BP3D_CUDA', parameters=None)
```

Code snippet 2. Reconstruction function examples of module *rec*.

3 Conclusions and future improvement

A tool for X-ray GI data analysis has been developed in the framework of the PRIN2022 PITCH Italian project, which involves several Italian academic and research institutes. The setup devised in the context of this project, designed for cultural heritage analysis, is capable of performing radiographic and tomographic analysis through phase stepping and Moiré acquisition methods. The data analysis routine is entirely developed in Python using set up Jupyter notebooks for the different tasks (signals extraction, CT reconstruction and visibility analysis). At present, only data taken with phase stepping can be analysed, but in the near future the system will be expanded to perform Moiré analysis as well, potentially more convenient in terms of acquisition time (especially for tomographic experiments). The signals extraction from radiographic analysis can be performed through two different methods—sine fitting and Fourier analysis, with the latter being devoted to signals extraction from tomographic data. CT reconstruction is based on ASTRA Toolbox algorithms (in particular for 3D geometry) with a different approach for differential phase contrast images, using a Hilbert transform kernel for images pre-filtering. Literature research and further tests on different reconstruction methods are carried on for possible improvements, as well as correction tools for tomographic artifacts (e.g., due to gratings imperfections) [16]. Future work will concern the development of a GUI and possibly also a web app to be shared with the scientific community, aimed at guaranteeing a more interactive and simpler approach for the users. The code package is not publicly available but is used only for the PITCH data processing at the moment; as soon as all the development tasks are completed and tested, the authors will be able to share it with the scientific community with the relative documentation.

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