AUTOMATED TOMOGRAPHIC ALIGNMENT OF LINEAR AND ANGULAR UNCERTAINTIES AND APPLICATION TO PHASE-CONTRAST DATA

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Summary: Phase-contrast X-ray tomography is a powerful quantitative high-resolution technique for nano-scale studies. Projection images must be subjected to alignment, background linear terms removal and phase unwrapping in order to preserve its quantitative properties. We present an automatic alignment and reconstruction technique insensitive to background linear terms and phase wrapping with optimization of all the linear and angular projection parameters.

1. INTRODUCTION

The introduction of coherent diffraction imaging (CDI) in tomography has allowed the acquisition of projection images with high spatial resolution (8–10 nm range) [1], for relatively large fields of view without the need for imaging lenses or optics. Besides its high spatial resolution, phase-contrast data produced by CDI techniques also provides a quantitative measurement of the refractive index of the sample under study that is directly related to its electron density distribution. This acquired micro and nano-scale information can be of high-interest in different material science applications especially for energy conversion and storage materials where the performance is determined by their internal structure. In order for 3D tomographic reconstructions (from phase-contrast projection data) to exhibit similar spatial resolutions and quantitative measurement accuracy, a proper projection alignment must be performed before tomographic reconstruction. Phase-contrast projection data presents additional properties that must be taken into account prior to tomographic alignment and reconstruction, such as the presence of background linear terms and wrapping areas characteristic of phase signals. Although phase unwrapping algorithms [2] can be applied to phase-contrast projection images these are usually time consuming, may require user interaction and can even generate undesired artefacts in the presence of noise or *unpaired phase residuals*. We propose an automatic tomographic alignment algorithm insensitive to phase wrapping and linear background terms, including a linear background term removal and a fine iterative optimization step where all angular and linear alignment terms that define a sample-detector relative orientation can be refined.
General or complex projection geometries (including tilt angles and uneven projections distribution) can be resolved by means of iterative algebraic tomographic reconstruction algorithms, such as SIRT, that we have extended to phase-contrast wrapped data with the possibility of excluding defective pixel information such as *unpaired phase residuals*, avoiding unnecessary unwrapping operations that could, as previously mentioned, be responsible for the introduction of undesired artefacts.

2. METHODOLOGY

The full proposed alignment and reconstruction algorithm is composed by three main steps:

- An initial coarse alignment for linear projection parameters, using cross-correlation techniques in the phase derivative domain (insensitive to phase wrapping and linear background terms)
- An automatic projection data normalization or background linear terms removal
- An iterative optimization of all the rigid body movement projection alignment parameters that describe any detector-sample relative orientation including both linear and angular parameters such as translations and tilt projection angles.

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3. RESULTS

- The results of our work will be presented for simulation data as a proof of concept of the proposed method and to several real data ptychography data acquired at the cSAXS beamline at the Paul Scherrer Institut (PSI), Switzerland.
- An example of application of algebraic iterative reconstruction algorithms for wrapped phase-contrast data is presented in Figure 1a. The introduced modification in the SIRT algorithm allows recovering an accurate tomographic reconstruction without previous sinogram unwrapping.
- Figure 1b illustrates a visible resolution increase in a tomographic slice after the optimization of tilt angular parameters. These results were quantified by means of Fourier shell correlation measurements, as shown in Figure 1c and other numerical residual metrics.

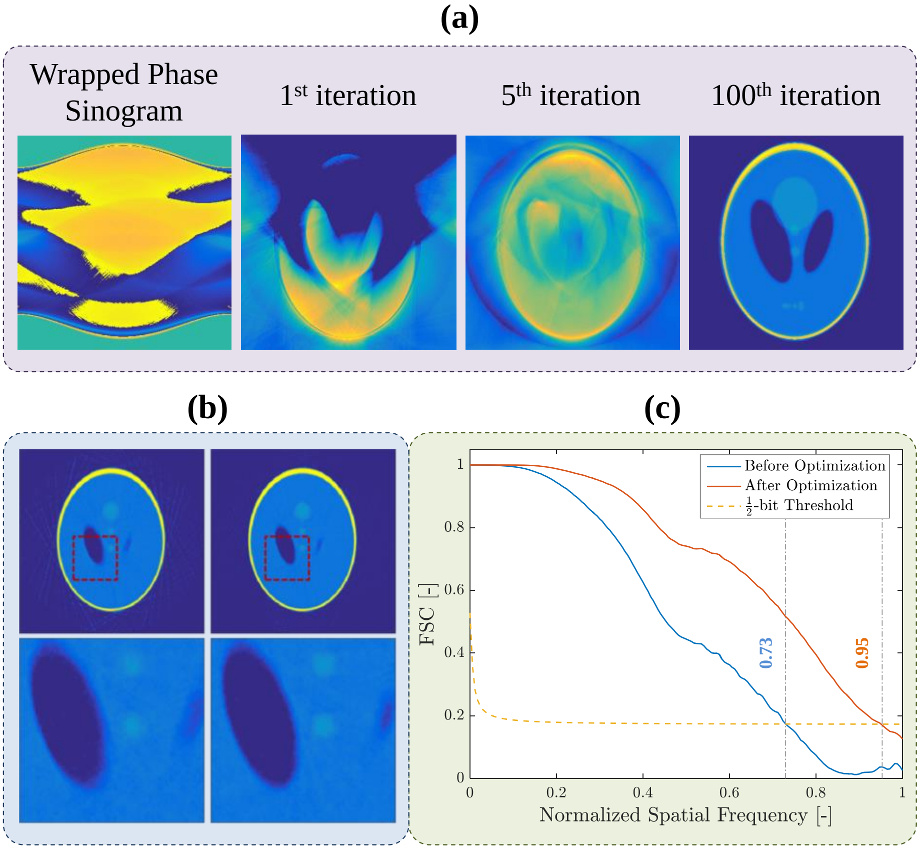

Figure 1: (a) Tomographic reconstruction evolution for different iterations of the proposed reconstruction algorithm. **(b)** Reconstruction resolution improvement and **(c)** Fourier Shell Correlation (FSC) quantification before and after linear and angular alignment parameters optimisation.

References

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