Fast Tomographic Alignment for Joint Ptychography and Tomography

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Abstract
Joint ptychography and tomography (JPT) is a recently developed framework that enables high-resolution reconstruction of 3D volumes with significantly relaxed constraints on probe overlap at adjacent scan positions. In ptychographic X-ray computed tomography (PXCT) experiment scanning translations are controlled with high-precision piezo-stages, while run-out errors of rotational stages are corrected by aligning phase-retrieved projections. However, such projections are by definition not available for JPT and would thus require precise knowledge of the angular positioning of the sample, which is prohibitively limited by hardware precision. Here, we present a method for correcting the misalignment of ptychographic tomography data with respect to the rotation axis without having to retrieve individual phase projections. This will facilitate development and application of JPT in providing fast data-efficient nanotomography experiments.

Introduction
X-ray ptychography is a powerful microscopy technique that has been successfully developed from the synergy of raster scanning and coherent diffraction imaging techniques [1], [2]. Ptychography provides unlimited fields-of-view and exploits phase retrieval algorithms to reconstruct the sample and the generally unknown illumination (probe) [3]. When applied in a computed tomography setting it has been able to achieve sub-15 nm isotropic 3D resolution of the reconstruction [4]. Conventional reconstruction of PXCT data implies a decoupled approach by first retrieving 2D projections and then uses them as an input for the tomographic reconstruction. Such decoupling is necessary for post-processing of retrieved phase projection prior to the tomographic reconstruction. Phase projections need to be corrected for undesired phase terms, wrapped phase, and phase artefacts. Afterwards, corrected phase projections have to be aligned with respect to rotation axis to correct for run-out errors of the tomography stage [5], [6].

In ptychography, quality of retrieved projections is highly dependent on the degree of probe overlap at adjacent scanning positions. When followed by tomographic reconstruction, this approach becomes data extensive and time consuming. Recently developed optimization algorithms [7]–[10] have shown that solving coupled ptychography and tomography problem can greatly relax probe overlapping condition without loss of the reconstruction quality. This is achieved by the support of the angular overlap of the probe from tomographic acquisition, and the more strict constraint of the coupled problem. So far, all the existing JPT algorithms rely on precise knowledge of angular and translation parameters of the sample. Reconstruction of experimental data under the JPT framework utilizes parameters obtained from a conventional PXCT reconstruction [8], [11]. However, for such a scheme JPT is redundant since conventional reconstruction is already achieved. To fully exploit the potential of JPT one needs to address post-processing procedures of conventional PXCT, that can be in principle done as a part of JPT optimization.
In this paper, we discuss a possibility of using methods of scanning transmission X-ray microscopy (STXM) [12], [13] for JPT. STXM data is already available from PXCT data (Fig. 1) and can yield projections of various contrast modes without phase-retrieval that can be used for tomographic alignment.

Figure 1. Schematic of PXCT/STXM set-up. The incoming X-rays are concentrated into a sharp beam using focusing optics and raster scanned across the sample. The diffraction signal is recorded at every scanning position with a far-field pixel array detector. Tomography is done by rotating the sample.

Contrast Mechanisms in STXM
A wave front transmitted through the specimen (or exit wave) at a given scanning position can be written as a product of the probe function $P(r)$ and the object function of the specimen along optical axis $z$, or explicitly:

$$\psi(r) = P(r - r_j) \exp\left[\frac{2\pi i}{\lambda} \int n(z) dz\right],$$

(1)

where $r - r_j$ is a current scanning position, $\lambda$ is the wavelength of the incident wave-front, and $n$ is the complex refractive index of the specimen. According to the Fraunhofer approximation, the intensity of the exit wave propagated onto the far-field detector is given by: [14], [15]

$$I(r - r_j) \approx \int |\mathcal{F}\{\psi(r - r_j)\}|^2 R(k) dk,$$

(2)

where $\mathcal{F}$ is the two-dimensional Fourier transform, $R(k)$ is the detector response function, and $k$ is a position in the detector plane. For the pixel array detector used in PXCT data acquisition, the function $R(k)$ can be defined computationally to recover different contrast modes from a single measurement [14], [16].

Figure 2. (a) Absorption projection. (b) Dark-field projection. Insets of the figures show masking of diffraction data.
The absorption contrast (AC) projection is obtained by mapping total intensity of the signal on the detector at a given scan position. This corresponds to uniform detector response $R(k) = \text{const}$. Dark-field contrast (DFC) projections are produced from taking into account only scattered signal [17]. This is done by masking the signal from the primary beam on the detector [18]–[20]. Fig.2 presents absorption and dark-field projections along with the corresponding masking of diffraction patterns. Practically, both AC and DFC can be enhanced by manually finding suitable detector response function $R(k)$ (mask). For example, as in Fig.2(a) masking the outer parts of the diffraction pattern effectively worked as a post-acquisition reduction the probe size that reduced blurring effect of the probe overlap. The projections are produced from PCT data that was acquired using the probe with a spot size of 1 µm that was scanned the sample across 16 µm by 12 µm field-of-view with around 20000 scanning positions per angular view.

Differential phase contrast (DPC) is another mode that can be derived from PXCT data by estimating deflection of the beam from the optical axis [21]. There are several advantages of DPC compared to conventional AC, such as stronger contrast [22] and superior signal-to-noise ratio at equivalent amount of radiation dose [23]. In addition, DPC is faster to calculate as it does not require manual choice of the optical mask and only coordinates of the optical axis has to be known. DPC is usually represented by two images, corresponding to orthogonal phase gradients, derived as:

$$G_x = \frac{l_l - l_r}{l_l + l_r}$$

where $G_x$ is the horizontal phase gradient, $l_l$ and $l_r$ are total intensities at the left and the right detector half-planes, respectively. Derivation of the vertical phase gradient $G_y$ follows the same procedure, but for the top and the bottom detector half-planes. Fig.3 shows components of the phase gradient and diffraction pattern half-planes used in the derivation.

$$G = \sqrt{G_x^2 + G_y^2},$$

Figure 3. (a) Horizontal phase gradient projection. (b) Vertical phase gradient projection. The red and blue rectangles inside of the insets depict corresponding detector half-planes used to derive phase gradient projections from diffraction data.

Absolute phase projection can be retrieved from DPC projections by various methods as direct integration, Fourier integration [16], [24], or iterative schemes [25], [26]. However, they can lead to projections with phase retrieval and wrapping artifacts. The artefacts will then propagate into the tomographic reconstruction and can potentially corrupt the reconstructed volume. Fig.4(a) shows an example of the phase projection reconstructed from phase gradients in Fig.3 using Fourier integration method available through the open-source Python package Wavepy [27]. The reconstructed projection was then corrected for the linear phase term. Constant phase offset and wrapping artifacts are still present in the phase projection and require additional correction. Another variant of DPC is the phase gradient magnitude (Euclidean norm) given simply as:
Fig. 4(b) shows the magnitude projection derived from phase gradients in Fig. 3. The phase gradient magnitude projection is insensitive to linear and constant phase terms. Moreover, it is free of phase-retrieval and phase wrapping artifacts across the complete area of scanning that makes it a perfect candidate to serve as an input for tomographic alignment. It can also be used for the region-of-interest reconstruction as the weight function that indicates the presence of the features within the scanned area.

**Tomographic Alignment of PCT Data**

Modern synchrotron ptychography/STXM beamlines are equipped with interferometer-controlled scanning stages with sub-10 nm positioning accuracy [28], [29]. A misalignment of projections with respect to the rotation axis may be present as tomography data is acquired independently for every angular view. The misalignment may arise from intrinsic limitations of a rotary stage (run-out errors), mechanical instabilities or thermal drifts due to long scanning time per angular view. Various methods have been proposed to correct for the misalignment of projections and were briefly discussed in [5]. For X-ray nanotomography the most common approach is based on the assumption that two neighboring projection are infinitely close to each other and alignment can be performed by sequentially cross-correlating adjacent projections [30]. In the first approximation, precision of such approach depends on the density of angular sampling and accumulated registration errors can propagate from one angular view to another. Vertical misalignment can be efficiently corrected by using so-called common-line method that estimates a distribution of the mass integrated along horizontal axis and tracks its fluctuation from projection to projection. Advantage of such method is that this fluctuation is completely independent of the horizontal misalignment and a sub-pixel precision can be achieved by cross-correlating integrated mass distribution at adjacent projections. More advanced alignment can be achieved using "bootstrapping" or "projection-matching" algorithms that are using the fact that all projections have to be consistent within the unique three-dimensional reconstructed volume [5]. However, solving alignment problems with such an approach comes with a higher computational cost compared to fast cross-correlation, since iterative re-projection schemes are exploited. Recently, a framework has been proposed that combines above methods and can achieve alignment with deep sub-pixel accuracy [31]. The framework implies sub-optimal alignment of projections by cross-correlation and common-line methods followed by multi-resolution alignment using iterative re-projection algorithms.

**Results and Discussion**

![Figure 4. (a) Phase projection reconstructed using Fourier integration method and corrected for linear phase term. (b) Phase gradient magnitude projection.](image-url)
For demonstration purposes of the proposed method, we performed tomographic alignment using an iterative projection-matching algorithm, suggested in [5] that is available through the open-source Python package for tomography analysis TomoPy [32]. Here, common-line and cross-correlation methods are used to highlight the difference between the original misaligned projections and projections aligned using the iterative re-projection algorithm. Although, the true values of the misalignment are not available for experimental data, such comparison can be used in studying the alignment with the proposed method. Fig.5 shows integrated mass distribution of projections before and after the alignment. Black horizontal grid lines are added to assist the comparison of vertical shifts between projections before and after the alignment. Fig.6 shows integrated mass distribution of projections before (a) and after (b) the alignment. Horizontal grid lines are shown in black for reference.

alignment. Fig.6 shows the horizontal component of the cross-correlation between adjacent projections before and after the alignment along with the convergence plot of the alignment algorithm over iterations. Convergence to sub-0.2 pixel error has been achieved in less than 30 iterations of the algorithm.

Conclusions
In this paper, we discussed the possibility of using STXM data to align PXCT data for JPT. Previously, STXM data was used to align and correct X-ray fluorescence tomography data for self-absorption effects [33], [34]. We have demonstrated that projections with alternative contrast modes can be obtained from diffraction data and used for the tomographic alignment. In particular, phase gradient magnitude projections provide a superior signal-to-noise ratio, as well as high contrast for edges of the sample and of internal features. Such projections do not require probe overlap and can be obtained without use of phase-retrieval algorithms. Therefore, reconstruction artefacts, phase offset, and phase wrapping
ambiguity do not affect them. In that case, the alignment can be done using the fully scanned area and not just well behaved regions. We believe that the proposed method will push the development and application of a new generation of data efficient JPT reconstruction algorithms for ptychographic nanotomography.

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