Abstract: Tomographic coherent imaging requires the reconstruction of a series of two-dimensional projections of the object. We show that using the solution for the image of one projection as the starting point for the reconstruction of the next projection offers a reliable and rapid approach to the image reconstruction. The method is demonstrated on simulated and experimental data. This technique also simplifies reconstructions using data with curved incident wavefronts.

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References and links


1. Introduction

Coherent diffractive imaging (CDI), that inverts a far field x-ray diffraction pattern to obtain a quantitative image is now a viable and useful technique [1–4]. At third generation synchrotron sources a rationale for this work lies in the promise of high resolution 3D microscopy for...
materials and biological samples. Since the first demonstration of CDI using x-rays [5] the technique has been applied to various isolated materials samples [6–8], as well as de-hydrated [9–11] and hydrated biological specimens [12, 13].

CDI uses iterative algorithms that recover the phase of the diffracted wavefield. A range of new algorithms continue to be developed [14]. A significant portion of this work is motivated by problems with stagnation, or the speed of the iterative solutions. Examples include algorithms such as hybrid input-output (HIO) [15] and difference map (DM) [16], which are argued to reduce the chance of stagnation by not strictly enforcing steepest descent [15]. “Pytchographic” methods incorporating multiple diffraction data sets based on a translated illumination have also shown notable improvements in reconstruction quality [17, 18].

The uniqueness of the recovered solution is also known to be compromised by certain pathological cases [19]. It has been shown that these problems can be ameliorated by use of sufficient phase structure in the illumination, often provided in the form of spherical curvature [20]. In this case, the resulting far-field diffraction pattern must be treated in the Fresnel approximation [20–22]. Experimental verification of this Fresnel coherent diffractive imaging (FCDI) approach has now been obtained [8, 11, 23–26].

In many experimental geometries, the complex exit surface wave from a sample obtained by CDI can be described as a projection through the sample [27]. In this case the Fourier slice theorem [28] can be used to calculate the 3D sample distribution from a series of angular projections.

In this paper we consider a method of 3D CDI phase retrieval in which the complex solution for the previous projection is used to start the iterative algorithm for the next projection. “Bootstrapping” each solution in this way leads to faster convergence for each projection. Using recovered phases as starting points for iterative reconstructions has been explored in 2D CDI [29]. Here we apply the idea to the 3D case and quantify the improvement. We conclude that under realistic conditions, bootstrapping will offer a significant speed advantage.

2. Method

The iterative reconstruction algorithms we use are based on the original ideas of [15, 30], and have been usefully summarised elsewhere [14]. In this paper we use FCDI with error reduction (ER) [31], in which the illuminating field is used to define the object extent [24]. The iterative algorithm was run until a self consistent, or converged solution was obtained. This was quantified by the $\chi^2$ between the simulated or measured data, $I(\rho_d)$, and the squared amplitude of the current iterate, $|\hat{\psi}(\rho_d)|^2$:

$$\chi^2 = \frac{\sum_{\rho_d} \left[ |\hat{\psi}(\rho_d)| - \sqrt{I(\rho_d)} \right]^2}{\sqrt{\sum_{\rho_d} I(\rho_d)}},$$  

where $\rho_d$ is the detector coordinate. Specifically, convergence was defined to be when $\chi^2$ between successive iterates differed by less than a defined fraction, $F$. Changes in experimental geometry, sample size, noise levels, and the defined support region can vary the $\chi^2$. Here we used a convergence of $F = 10^{-4}$ for the simulations and $F = 10^{-3}$ for the experimental data.

Our method, which we term the “bootstrap” method, is as follows. Given a recovered transmission function for a neighbouring projection, $T_{\theta-\Delta\theta}$, and the measured or simulated intensity at the detector, $I_{\theta}$, an initial estimate for the wavefield at the detector for the current projection, $\hat{\psi}_{\theta}$, is calculated via:
ψ_\text{e}(\rho_d) = \int_{\rho_s} \psi_0(\rho_s) T_{\theta-\Delta\theta} e^{i \frac{\pi \rho_d^2}{2 z_D}} e^{-2\pi i \rho_s \rho_d} d\rho_s ; \text{ and} \tag{2}

ψ_\theta(\rho_d) = \sqrt{I_{\theta}(\rho_d)} \left| \frac{\hat{\psi}_\text{e}(\rho_d)}{\hat{\psi}_\text{e}(\rho_d)} \right|. \tag{3}

Here \( \rho_s \) and \( \rho_d \) are the 2D sample and detector coordinates respectively and \( \psi_0(\rho_s) \) is the illuminating beam in the sample plane. \( \hat{\psi}_\text{e}(\rho_d) \) is the initial estimate of the sample exit wavefield propagated to the detector using the Fresnel free space propagator [23] with a propagation distance of \( z_D \), and wavelength \( \lambda \). This is then iterated on using the techniques of 2D FCDI [8, 26].

The recovered complex exit surface wave is used to obtain the projection through the sample of both the decrement from unity of the real part of the refractive index, \( \delta \), and the imaginary part of the refractive index, \( \beta \) [32]. Standard methods of filtered back projection [33] can then be used to obtain the 3D distribution of either quantity.

We now provide simulation and experimental results showing that 3D reconstructions can be successfully obtained using this approach, and quantify the increase in convergence speed.

3. Simulations

In order to explore the reconstruction methods, the geometry and parameters from a typical FCDI x-ray experiment were used [see Fig. 1 (left)]. A single element 3D object was analytically created for simulation purposes. The object represents a glass capillary used as a tomography sample mount in x-ray experiments. The large phase contrast between glass and carbon (an order of magnitude in \( \delta \) at the energies explored in this paper) is also desirable. The simulated capillary is modelled on an FCDI reconstruction of the projection of an actual fractured capillary [Fig. 2(a)] obtained using the setup and method described in [26]. The corresponding 3D analytical model and its projection are identical to the eye in this reconstruction, shown in Fig. 2(b) and 2(c). The capillary has a diameter of 3\( \mu \)m and a wall width of 400\( \text{nm} \).

The complex refractive index for the simulated object was taken from [34] at an x-ray energy of 2.54keV, assuming a composition of Schott 8092 glass [35] with a density of 3.01g/cm\(^3\) .

The 2D phase and amplitude of the sample exit wavefield for a given projection, \( \psi_{\text{e, } \theta}(\rho_s) \), in the projection approximation [27] were obtained using:

\[
\psi_{\text{e, } \theta}(\rho_s, z_S) = T_\theta(\rho_s) \psi_0(\rho_s, z_S),
\]

where \( \rho_s = (\rho_s, z_S) \) are the coordinates in the exit plane of the sample. \( T_\theta(\rho_s) \) describes the complex transmission function of the object for the current projection angle as a function of the

<table>
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<tr>
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<td>Detector Pixel Width:</td>
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Fig. 1. Experimental Parameters.
Fig. 2. (a) Amplitude of the transmission function of an actual glass capillary reconstructed from an FCDI tomography data set. This dataset was used to define the parameters for the simulated data set used in this study. (b) Projection through the 3D reconstruction of the simulated capillary used throughout this study, showing the amplitude of the transmission function. The colour scale in both (a) and (b) represents x-ray transmission from 50% (blue) to 100% (white). (c) 3D reconstruction of the $\delta$ component of the refractive index, sectioned to display the central region. (d) and (e) Slices through the reconstructed glass capillary for the $\delta$ and $\beta$ components of the refractive index. The red box indicates the regions from which the components were averaged.

$3D$ complex refractive index $n(r_s) = 1 - \delta(r_s) + i\beta(r_s)$. Using appropriate coordinate transformations:

$$T_\theta(\rho_s) = \exp \left[ \frac{k}{2i} \int_{z_p} [1 - n^2(\rho_s, z_p)] dz_p \right].$$

(5)

Various “multi-slice” methods [36–38] for calculating the exit surface wave of an illuminated object were explored. These build on the projection method in a slice by slice fashion. However, for the geometry in these, and other typical FCDI experiments, there was no significant difference between the “multi-slice” approximations and the exit surface wave obtained under the projection approximation.

Exit surface waves for different projections of the sample were calculated at 1° increments between $\pm \frac{\pi}{2}$. The resulting exit surface waves were then propagated to the far field using the paraxial Fresnel free space propagator in Eq. (2). All phase information was then discarded in obtaining the squared amplitude of the diffracted wave, $I_\theta(\rho_d) = |\hat{\psi}_\theta(\rho_d)|^2$, as would be the case in a typical CDI experiment.

100 frames of data for each projection were simulated by injecting random fluctuations into the diffraction data based on statistics observed in previous experimental data [8, 24, 25, 32]. A single frame of FCDI data obtained under our typical experimental conditions [26] at 2-ID-B at the Advanced Photon source is a 1 second exposure containing order 500 photons per pixel in the central holographic region. This number falls off rapidly for the high angle coherent scatter. These 100 frames were averaged to create a final simulated diffraction pattern, whose noise levels were in good agreement with the Poisson statistics observed in experimental data. A study of the various types of noise and its effects on CDI reconstructions has been performed elsewhere [39].

Reconstructions were performed on the complete dataset using the method described in Section 2. Figure 3(a) shows the advantage of bootstrapping using the reconstruction of the $n^{th}$ projection as a starting guess for the $(n+1)^{th}$ projection. The dashed lines in Fig. 3 show the number of iterations required for the $\chi^2$ error metric to converge ($F \leq 10^{-4}$) between succes-
Fig. 3. (a) The number of iterations required to reach a self-consistent solution at the $1.0 \times 10^{-4}$ level in simulated data. (b) Iterations required to reach a self-consistent solution at the $1.0 \times 10^{-3}$ level during reconstructions of the insect wing.

sive iterates. The solid lines indicate the number of iterations required for each projection when using the bootstrap method. Figure 3(a) shows up to a $10\times$ speed increase for the total 3D reconstruction time, even in the presence of experimental noise.

Slices through the $\delta$ and $\beta$ components of the reconstructed object obtained using the bootstrap method are shown in Figs. 2(d) and 2(e) respectively. The recovered values, tabulated in Fig. 4, show the bootstrap and standard methods to be quantitatively very similar. The recovered values are also in good agreement with the actual values.

Similar results in speed up and quantitative recovery of the refractive index have been obtained for other objects, including those that are non-cylindrically symmetric and are composed of multiple materials.

4. Optical Experiments

Experimental FCDI tomography data was collected using coherent monochromatic focused ($NA = 19.6$) optical laser light using the experimental parameters in Fig. 1 (right). The focused beam illuminated the wing tip of an insect [see Fig. 5(c)] with a field of view of approximately $1 \text{mm}^2$. 25 frames of diffraction data, each 1 second long were taken for each projection between $\pm \frac{\pi}{2}$, at $\frac{\pi}{5}$ increments. This provided a high enough signal to noise for scattered photons to be measured at the edge of the detector array [see Fig. 5(a)]. Reconstructions were performed using the method described in Section 2.

A single projection through the 3D reconstruction is shown in Fig. 5(b), with the rendered 3D reconstruction in Fig. 5(d). An obvious likeness can be seen with the corresponding optical microscope image shown in Fig. 5(c). The differences in the appearance of the wing tip between Figs. 5(b) and 5(c) are due to artifacts in the FCDI reconstruction. A contributing cause of these artifacts is specular reflections from the surface of the wing.

Notwithstanding these issues, the bootstrap process is shown in Fig. 3(b) to provide a com-

\[
\begin{array}{ll}
\delta_{\text{Glass}} & \beta_{\text{Glass}} \\
\text{Actual} & 7.32 \times 10^{-5} \\
\text{Standard} & (7.5 \pm 0.2) \times 10^{-5} \\
\text{Bootstrap} & (7.7 \pm 0.3) \times 10^{-5}
\end{array}
\]

Fig. 4. Average reconstructed values for the x-ray simulation in the regions indicated in Fig. 2(d) and 2(e). Errors are calculated from the standard deviation of the region of interest.
Computational advantage. An improvement by a factor of \( \sim 2 \) is observed compared to the standard method. At the same time the reconstruction quality was not compromised.

5. Computational Bootstrap Benefits

The relative advantages of 3D CDI and the bootstrap methods can be quantified by considering the amount of memory, and the order of the number of operations required to obtain a reconstruction. We also consider the curved beam analogue of 3D CDI, namely 3D FCDI. To date 3D FCDI has not been demonstrated; here we consider what the load may be should the technique be elucidated.

If \( N = 2048 \) is the linear dimension of the detector array, then the 3D complex diffraction volumes for 3D CDI and 3D FCDI would occupy 296 GB of RAM. In our case the bootstrap FCDI code requires less than 1 GB, corresponding to the measured diffraction data and illumination for a single angular projection.

To gauge the computation time for each method we make the assumption that the number of operations to complete a single FFT is \( O(N^d \log_2 N^d) \) (where \( d \) is the dimensionality of the transform), and operations such as applying a support or a modulus constraint are \( O(N^d) \). We also assume that convergence is obtained in \( M \) iterations. Using \( P \) angular projections a 3D CDI reconstruction uses two 3D FFT’s and a support and modulus constraint for each iteration, and would thus take of the order of \( 2M \times N^3 (3 \log_2 N + 1) \) operations. In 2D FCDI

\[
\text{Computational Order} \\
\begin{array}{c|c}
\text{3D CDI} & 2M \times N^3 (3 \log_2 N + 1) \\
\text{3D FCDI} & 2M \times N^3 (3 \log_2 N + 2) \\
\text{Bootstrap FCDI} & 2M \times N^2 (2 \log_2 N + 2) (1 + \frac{P-1}{N}) + P \times N^2 (N + 2 \log_2 N + 1)
\end{array}
\]

\[
\text{Calculated Operations} \\
\begin{array}{c|c}
\text{3D CDI} & 3 \times 10^{14} \\
\text{3D FCDI} & 3 \times 10^{14} \\
\text{Bootstrap FCDI} & 5 \times 10^{12}
\end{array}
\]

Fig. 6. The nominal number of computational operations used in various 3D reconstruction techniques.
the curvature in the illuminating wavefield is sequentially added and subtracted from the iterate during each cycle of the algorithm [8, 32]. The same approach can be taken in the 3D case, at a cost of \( O(N^3) \) operations every iteration. Accordingly, the 3D FCDI reconstruction would take of the order of \( 2M \times N^3(3\log_2 N + 2) \) operations. The bootstrap FCDI method requires two FFT’s, a support and a modulus constraint, and addition and subtraction of the illuminating wavefield for each iteration. This is then repeated after the first projection for the remainder of the \( P \) projections, taken at a speed up factor of \( S \) due to the use of the previous solution as a start guess. In addition, a single 3D filtered back projection step (order \( P \times N^2(N + 2\log_2 N + 1) \) operations) is required to repeat the 3D reconstruction. Consequently, of the order of \( 2M \times N^2(2\log_2 N + 2)(1 + \frac{P-1}{S}) + P \times N^2(N + 2\log_2 N + 1) \) operations are required for bootstrap FCDI.

In a typical FCDI tomography reconstruction \( N = 2048 \) and \( M = 500 \). While the optimal number of angular projections to reconstruct an object spanning \( N \) pixels using filtered back projection is \( \frac{\pi}{2}N \) [40], we assume \( P = 180 \) as a more experimentally attainable number. Using these figures, and assuming an \( S = 5 \times \) speed increase for bootstrapped projections leads to the total number of operations described in Fig. 6.

6. Conclusion

Using simulations and experimental data we demonstrated that the bootstrap method can provide significant computational advantages in FCDI tomography, which can be extended to the plane wave geometry of CDI. These advantages may be a speed increase of the order of \( 10 \times \). This figure can be even higher, for instance when providing multiple seeds to the set of reconstructions, or in the case of small angular steps or high object symmetry. The memory and storage overhead of the bootstrap method is also far less than the direct 3D methods, allowing it to run on a single processor desktop computer while still obtaining 3D reconstructions for large arrays. A further advantage of FCDI tomography is the ability to image objects which extend beyond the illumination in the vertical direction. In 3D CDI this is complicated due to the requirement for finite object support. Objects that are large laterally can also be imaged using the ptychography approach [41]. This will further increase the size of the data set involved and increase computation times. The combination of bootstrapped tomography with ptychography will greatly reduce the total computational time required to obtain high quality 3D reconstructions.

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