Astigmatic phase retrieval: an experimental demonstration

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Abstract: We present the first experimental demonstration of the astigmatic phase retrieval technique, in which the diffracted wavefield is distorted by cylindrical curvature in two orthogonal directions. A charge-one vortex, a charge-two vortex, and a simple test image are all correctly reconstructed.

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References and links

1. Introduction

Coherent Diffractive Imaging (CDI) is a method of lensless imaging in which an image is reconstructed from the diffraction pattern of the sample. The spatial resolution in the reconstructed image is limited only by the wavelength of the illumination and the maximum angle at which diffraction can be reliably detected. The recent development of X-ray free electron lasers allows for the possibility of using CDI for very high resolution X-ray imaging, possibly permitting the imaging of single biomolecules [1,2].

CDI has now been shown to be a successful imaging method and has been applied to image single biological cells [3,4], the strain distribution in single crystals [5], ceramic nanofoams [6] and integrated circuits [7]. However, in spite of its success, the method can be difficult to implement, the iterative methods may not always converge and, initially, was only applicable to finite objects. Many of these problems have been mitigated by the introduction of phase curvature to the illumination [8–10], or methods such as ptychography [11,12] and related data analysis techniques [13].

The abovementioned techniques are showing themselves to be very powerful, however, it is well-established that they all have uniqueness problems to some degree. For example, CDI has been established as being incapable of distinguishing homometric structures — distinct
structures that produce identical Fraunhofer diffraction patterns – as well as the so-called trivial ambiguities identified by Bates [14]: translation, inversion, conjugation and phase-offset. Fresnel diffraction uniquely defines the object to within complex conjugation [15]. The aim of this paper is to demonstrate the implementation of a method, astigmatic phase retrieval [16], that is truly unique, by reconstructing the phase of a single axially-symmetric optical vortex [17].

The optical vortex contains a point discontinuity in its phase distribution and the phase accumulates by an integer multiple of $2\pi$ around the discontinuity, where the integer is referred to as the topological charge. None of the existing phase recovery methods can correctly recover the phase distribution of a single axially-symmetric phase vortex, including its handedness.

The existence of optical vortices demonstrates that a light wave can carry both linear and angular momentum [18] and a formalism for the meaning of phase has been developed that makes this explicit [19]. It follows from simple information-theoretic arguments [20] that defining the energy flow of the field through space requires a minimum of three measurements, a condition obeyed by the astigmatic phase retrieval approach. While the through-focal method [21–23] meets that criterion, these methods do not include a characterizable symmetry-breaking operation and so cannot, in principle, reliably resolve the sign of the topological charge of a single axially-symmetric phase vortex.

The controlled use of phase aberration has been widely used in both the optical and electron microscopy fields, where a known wavefield is interfered with the unknown wave of interest. This method forms the basis of holography techniques, and more recently, digital Fourier holography [24], where the illuminating field is computationally added and subtracted from the combined field. Knowledge of the illuminating phase profile has had extensive use in aberration correction of optical systems, such as electron microscopes [25], the Hubble space telescope [26], and more recently, the substitution of physical optics by computational methods [27] where the phase recovery process is referred to as “phase-diverse phase retrieval.”

The method we present makes use of the addition and subtraction of a known cylindrical phase distortion which removes the sign ambiguities of the vortex by using symmetry-breaking lenses, thereby providing a truly unique solution for the phase of the wave. The idea of cylindrical symmetry-breaking structures has origins in the method of phase-space tomography [28] and astigmatic diffraction has also been considered for application to electron imaging [29], an area in which the role of electron vortices has been examined in some detail [30,31]. This paper presents an experimental demonstration of phase retrieval using the method of astigmatic diffraction, correctly recovering the phase distribution from a discontinuous optical phase structure – a single axially-symmetric phase vortex.

Section 2 is a brief review of the theory underlying the astigmatic phase retrieval method; followed by discussion of the more general Gerchberg-Saxton-Fienup phase retrieval method, and a detailed outline of the implementation of the astigmatic method presented in this paper. In Section 3 we describe an experiment in which astigmatic phase retrieval data can be acquired in the visible-light regime. Section 4 presents results from three experimental wavefields: a charge-one vortex, a charge-two vortex and a simple test pattern. The paper is summarized and conclusions are presented in Section 5.
2. The theory of astigmatic phase retrieval

2.1 Theoretical background

The uniqueness of phase recovery algorithm model based on the paraxial wave equation has been analysed using the transport of intensity equation [17]. This algorithm continues to be of relevance here because iterative methods construct solutions of the paraxial wave equation, and we are here not so much interested in the method of solution as we are in the nature and existence of such solutions. It has been proven [17] that the phase recovery is unique, provided that the intensity is everywhere positive [17]; the presence of intensity zeroes allow for the possibility of phase discontinuities leading to phase ambiguities in the reconstruction.

It has also been argued [17] that introducing an astigmatic optical element breaks the cylindrical symmetry of the Fresnel propagator, allowing for a unique solution of the phase problem [16].

The change in the intensity distribution following a differential cylindrical distortion can be written as a directly soluble one-dimensional version [16] of the transport of intensity equation [32] – that is itself simply a statement of the conservation of energy on propagation for paraxial electromagnetic waves – which we write here as

$$k_0 R_x \Delta I_x (\rho) = \frac{\partial}{\partial \rho_x} \left[ I(\rho) \frac{\partial}{\partial \rho_x} \Phi(\rho) \right],$$

where $\rho = (\rho_x, \rho_y)$ denotes position in the far-field, the light has an intensity distribution $I(\rho)$, wavenumber $k_0$ and phase $\Phi(\rho)$, and changes by an amount $\Delta I(\rho)$ when the incident light is changed from planar to having a large radius of cylindrical curvature $R_x$ in the x-direction. An analogous expression exists for curvature in the y-direction. This expression offers a direct proof that two small orthogonal cylindrical distortions to the illumination are sufficient to uniquely define the phase and amplitude of the coherent wave [16]. Moreover, it was shown that if any phase discontinuities could be located, then these data could be directly integrated to recover the phase distribution.

In practice, a large incident curvature will provide a more easily measured experimental signal $\Delta I_x (\rho)$, the measurement no longer strictly satisfies the differential phase change condition inherent in Eq. (1), and a direct numerical solution is not possible using the methods described here. These conclusions are based on fundamental properties of paraxial Helmholtz waves, and are independent of the method of solution.

Uniqueness also seems likely for non-differential astigmatic distortions, but was not directly proven; however the reliability of the reconstruction was demonstrated using simulated data [16] and iterative methods.

2.2 Data analysis methodology

In the work presented here, we use an iterative approach to reconstruct the diffracted wavefunction of a sample. This is achieved by iterating three wavefunctions between two planes – the lens plane and the detector plane. This method is analogous to the iterative methods of the Gerchberg-Saxton-Fienup group of algorithms [33,34]. However, G.S.F. algorithms require the explicit imposition of a priori knowledge of the sample – information which can then be introduced to the algorithm to constrain the reconstruction to a solution – particularly information regarding the size of the sample via application of a pupil function as a support constraint [34].

By having three measurements of the intensity of the diffracted wavefunction at the detector-plane, our algorithm becomes over constrained, and thus we do away with the requirement for the explicit imposition of sample-plane constraints. Our algorithm, outlined in Fig. 1, is similar in regard to algorithms developed for through-focal series phase recovery [30]. The algorithm begins with some initial wave ($L_{\text{START}}$) at the lens plane. This could be a
realistic estimate of the sample’s exit surface wave propagated a distance \( l \) to the lens plane, for example, or it could be completely random.

From this, two further waves are created by incorporating the known cylindrical phase (\( \Phi \)) imposed by the two orientations of the cylindrical lens (\( x \) and \( y \)). This is achieved by multiplying the complex wavefunction by the phase distribution of an ideal thin cylindrical lens. The extent of curvature is calculated from experimental parameters, as follows,

\[
\Phi = -\pi x^2 / \lambda f ,
\]

where \( x \) is the displacement from the optical axis pixel, \( \lambda \) is the wavelength, and \( f \) is the focal length of the lens.

![Fig. 1. The steps of the algorithm. The wavefunctions at the lens plane (L) and at the detector plane (D) are modified by the functions between, which are explained in the accompanying text. Arrows indicate the order of the functions.](image)

These three waves (\( L_o, L_X, L_Y \)) are kept separate and are independently propagated to the detector plane by a Fourier transform (FT), generating three detector-plane waves (\( D_o, D_X, D_Y \)). The modulus constraint (Mod) is imposed, that is, the magnitude components of the three waves are each replaced with a new magnitude, obtained from their respective experimentally recorded intensities. The three new detector-plane waves (\( D'_{o}, D'_{X}, D'_{Y} \)) are then each Fourier transformed (FT\(^{-1}\)) back to the lens plane.

Two of the waves contain curvature (\( L'_o, L'_Y \)), representing the phase aberration imposed by the lens in the experiment. This curvature, added at the forward propagation stage, is removed (\( \Phi^{-1} \)) to produce three updated estimates of the wave (\( L''_o, L''_o, L''_o \)) from which a single updated estimate is obtained, via a simple arithmetic average [30]. A pupil function type support may be applied to this wavefield, if required, and the resultant wave is injected back into the iterative loop. No further assumptions about the nature of the interaction between the light and the sample are made, and in general we don’t apply a support, unless otherwise stated.

The iteration continues until the difference between the generated and experimental magnitudes of the detector-plane waves, the error metric, \( \varepsilon \), reaches some pre-determined target value or ceases to reduce in value. The error metric plays no explicit role in the algorithm – it simply monitors progress, and we use an error metric for the \( p^{th} \) iteration of the algorithm, \( \varepsilon(p) \) defined by

\[
\varepsilon(p) = \frac{1}{N^2} \sum_i \left( I_i - \hat{I}_i^p \right)^2 ,
\]

where a frame of data contains \( N \) pixels, \( I_i \) is the measured intensity in the \( i^{th} \) pixel and \( \hat{I}_i^p \) is the intensity in the \( i^{th} \) pixel at the \( p^{th} \) iteration.

As with other phase-recovery approaches, the final result is not a reconstruction of the sample \textit{per se}, but rather, it is a reconstruction of a wavefunction, which – in this case – is at

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the lens-plane. In keeping with convention, however, we will refer to the output as ‘the reconstructed sample’.

![Fig. 2. (a – c) Generated diffractive intensities on a 256 × 256 pixel array with: (a) horizontal curvature, (b) no curvature, and (c) vertical curvature; (d) the 100 × 100 pixel test sample used to generate the diffractive data, and (e) reconstruction at the 3000th iteration of the algorithm (Media 1), using a 110 × 110 pixel square pupil function as a support.](image)

The algorithm was tested using simulated data. Figure 2 shows a test object, and its far-field plane wave and orthogonal astigmatic diffraction patterns. Shot noise was added to the diffraction data, and reconstructions were obtained for a range of simulated exposure times. In this figure, each diffraction pattern contained a total of $1.3 \times 10^5$ photons with the brightest pixel containing $2.7 \times 10^2$ photons. The reconstruction of the sample was obtained with the use of a square pupil support and is shown in Fig. 2(e); (Media 1). The reconstructed intensities of the diffractive data very closely resemble the experimental intensities, and hence are not shown.

3. Experimental arrangement

Three test waves were created: a charge-one vortex, a charge-two vortex, and a non-vortex sample designed to test whether astigmatic phase retrieval can reliably reconstruct a more complex structured wave, consisting of an array of apertures.

A schematic of the experiment is shown in Fig. 3. Light from a fibre coupled laser diode (Thorlabs S1FC635) of wavelength 635nm is collimated with a microscope objective (20 × , NA = 0.4). Absorptive optical filters were used to prevent saturation of the CCD detector. For the vortex samples, the filter had a nominal neutral density of 2.0 and the diffraction data was detected with a Princeton Instruments VersArray 1300B CCD detector, 1340 × 1300 array with pixel size 20μm, cooled to −18.0°C. For the aperture sample, the beam was passed through a Thorlabs neutral density filter with OD = 1.0 and the data was detected with an Apogee Instruments Inc. U2000 CCD detector, 1600 × 1200 array with pixel size 7.4μm, cooled to −20.0°C.

For the experiments with an optical vortex, the parameters $l = 500$mm and $z = 620$mm were used. For the test aperture, the parameters $l = 60$mm, $z = 600$mm were used. Thorlabs BK7 plano-convex cylindrical lenses of focal length $f = 1000$mm (vortex samples) and $f =$
400mm (aperture sample) were placed after the sample to apply weak cylindrical curvature to the diffracting wavefield.

![Diagram of experimental setup](image)

Fig. 3. The set-up for the experiments; where $l$ is the distance between the hologram or sample and the lens, and $z$ is the distance between the exit surface of the lens and the CCD chip in the camera, and $f$ is the focal length of the lens.

Vortex waves with topological charge $m$ can be created by passing a uniform wavefield through a hologram with an amplitude transmission function as shown in Fig. 4(a) [35]. Transmission structures for $m = 1$ and $m = 2$ were created by printing on photographic film at a resolution of 1613 × 1613 pixels per cm$^2$. A structure of this form creates many orders, the 0th order representing the transmitted beam and the higher orders containing vortices with charge $\pm nm$, where $n$ is the order number and $m$ is the charge created in the first diffracted order. We define the vortices used in these experiments as having positive charge.

![Image printed onto hologram](image)

Fig. 4. (a) Image printed onto hologram used to create the charge-two vortex; (b) Simulation for testing the quality of the reconstructed charge-two vortex.

For each diffracting screen, the order of interest was recorded at a sufficient propagation distance such that all the orders were well separated, and that only the order of interest fell within the imaging window. The phase of a simulated charge-two vortex structure from a Gaussian incident beam with spherical phase curvature is shown in Fig. 4(b). It is the spherical phase curvature which gives the characteristic sigmoidal shape to the vortex, the rotational direction of which is a direct indication of the helicity of the vortex.
4. Experimental results

Once acquired, the data sets were centred with respect to each other by eye, by overlaying them as transparent layers with the GNU Image Manipulation Program [36]. A 512 × 512 pixel selection, set around this central pixel, was taken as the data array which was then rescaled to 256 × 256 pixels via a cubic interpolation, using the same program. This resampling was performed in order to reduce the computational time of the reconstruction process. Figure 5 shows the data set for the three conditions: (a) vertical cylindrical lens in place; (b) plane wave incident; and (c) horizontal cylindrical lens in place. The distortion due to the cylindrical lens is very obvious. Note also the asymmetric distortion of the intensity zero, a feature that enables the sign of the topological charge to be determined by the algorithm.

![Fig. 5. Experimental diffraction data of a charge-one optical vortex. Where: (a), (b) and (c) are the recorded intensities of the three propagated wavefunctions.](image)

A number of start guesses were used to begin the algorithm, including vortices with the incorrect charge (sign and/or magnitude), a plane-wave, and a set of random numbers. It was found that all succeeded in producing an excellent reconstruction; indeed the data was so strongly constrained that there was no need to impose a support constraint on the data. Figure 6 shows the phase of the wavefield recovered using a random start guess at the 150th iteration of the algorithm (Media 2). The error metric continued to reduce until around the 200th iteration, after which no significant improvement was seen. The vortex structure is obvious in the region where the amplitude is non-negligible.

![Fig. 6. Reconstructed charge-one vortex from a start function of random numbers. Displayed is the phase of the averaged reconstructed wavefunction, at the lens plane (Media 2).](image)

The vorticity of this reconstruction was measured by numerically integrating the phase gradient along a single square path, centered on the reconstruction. The total accumulated phase along a closed continuous path around the core of a vortex must equal $2\pi m$, where $m$ is the charge of the vortex. In this case, the charge was found to be 0.97 at the 150th iteration,
confirming our recovery of a charge-one vortex, where the discrepancy is due to numerical errors in integrating around the path.

The recorded intensities were horizontally flipped in order to emulate the imaging of a charge-one vortex of opposite handedness. Using the same random array as a start function and without the use of a support, a reconstructed vortex of opposite but equivalent charge, with calculated vorticity of $-1.02$, was obtained.

The data obtained for a charge-two vortex from experimental diffraction data are shown in Fig. 7. The reconstruction obtained from a random start and without the use of a support is shown in Fig. 8 (Media 3).

As with the charge-one data, the recorded intensities were horizontally flipped in order to simulate the imaging of a charge-two vortex of opposite handedness, using the same random array as a start function and without the use of a support, a charge-two vortex of opposite handedness was produced. At the 200th iteration, the calculated charges are 2.03 for the original data and $-2.13$ for the flipped data.

Comparison of the reconstructed charge-two vortex with the test pattern shown in Fig. 4(b), shows that it is not in fact a true charge-two vortex, but rather two closely spaced charge-one vortices. The diffracted waves which have undergone cylindrical distortion (Figs. 7(a) & (c)) clearly show two separated charge-one vortices, as expected for high-charge vortices in the presence of cylindrical astigmatism; but interestingly, the reconstruction from the algorithm shows that the lens-free (distortion-free) vortex (Fig. 7(b)) is also ‘split’: a fact which is not apparent by observation of the intensity distribution of the lens-free diffraction pattern alone. This observation is consistent with studies that show that higher charge vortices are rarely stable [37], and will split in the presence of even a minor perturbation. In experiment, any hologram used to create vortices will have minor imperfections, which
themselves can be cause for high charge vortices to split, and it is to this that we attribute the observed vortex splitting.

A non-vortex sample was imaged, consisting of 5 holes drilled into a 0.6mm thick black plastic sheet. The three recorded diffractive intensities are shown in Fig. 9.

Within 80 iterations of the algorithm, a reconstruction of the sample was achieved from a random starting guess, shown in Fig. 9(e) (Media 4). The reconstructed intensities of the diffraction data very closely resemble the experimental intensities, and hence are not shown. A 45 × 45 pixel square pupil function was applied as a support constraint for the first iteration only, without which the algorithm stagnates at an incorrect solution. Using the numerical aperture of the diffraction data, the reconstruction has a theoretical minimum resolution of 123µm.

Fig. 9. Experimental diffraction data from an array of apertures. Where: (a), (b) and (c) are the recorded intensities of the three propagated wavefunctions. (d) Microscope image of the sample and (e) with it blurred to have a resolution comparable to the expected best resolution possible from the diffraction data. (e) Intensity of the reconstructed wavefunction at the lens plane (Media 4).

An optical microscope image of the sample, shown in Fig. 9(d), was rescaled and convolved with a Gaussian function of a width calculated so as to mimic the effective numerical aperture of the reconstructed diffraction pattern. The blurred microscope image and the reconstructed sample are presented in Figs. 9(e) and (f) respectively. The lower right hand aperture has an approximate reconstructed width of 385µm, calculated by multiplying the number of pixels of the reconstructed pin-hole with the calculated sample plane pixel size from experimental parameters. This is in agreement with the measured width of 392µm for the same hole, measured with the optical microscope. The accuracy of the placement and proportions of the holes with respect to each other in the reconstruction is clear.

We have presented a new algorithm for iteratively reconstructing the phase profile of a sample from intensity recordings of its diffracted wave. By the imposition of orthogonal cylindrical curvatures onto this diffracted wave, a unique solution is obtained.

The case of an on-axis optical vortex was used to demonstrate the ability of the algorithm to provide a unique solution. Successful reconstructions of both the charge-one and charge-two vortices were achieved, without the use of a support. Calculation of the charge of the reconstructed vortices showed excellent agreement with the known charges.
The method was applied to experimental data from an aperture-type sample, demonstrating the effectiveness of the algorithm as a more general powerful imaging method. Excellent agreement between the reconstruction and microscope image of the sample was shown.

The application of cylindrical astigmatism for obtaining unique reconstructions by iterative phase retrieval has been shown to be a robust and fast imaging method. It has been demonstrated that it manages to obtain convergence even in the challenging case of a single axially-symmetric phase vortex.

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