Phase retrieval with the transport-of-intensity equation in an arbitrarily shaped aperture by iterative discrete cosine transforms

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A transport-of-intensity equation (TIE)-based phase retrieval method is proposed with putting an arbitrarily shaped aperture into the optical wavefield. In this arbitrarily shaped aperture, the TIE can be solved under nonuniform illuminations and even nonhomogeneous boundary conditions by iterative discrete cosine transforms with a phase compensation mechanism. Simulation with arbitrary phase, arbitrary aperture shape, and nonuniform intensity distribution verifies the effective compensation and high accuracy of the proposed method. Experiment is also carried out to check the feasibility of the proposed method in real measurement. Comparing to the existing methods, the proposed method is applicable for any types of phase distribution under nonuniform illumination and nonhomogeneous boundary conditions within an arbitrarily shaped aperture, which enables the technique of TIE with hard aperture to become a more flexible phase retrieval tool in practical measurements.

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Phase is not easy to directly detect as the intensity by energy-based sensors, but sometimes it contains the really desired information. In optical metrology, phase retrieval is a well-known terminology for either optical fringes [1] or optical wavefield [2]. As one important class of the noninterferometric propagation-based phase retrieval techniques for optical wavefield, the transport-of-intensity equation (TIE) [3] has gained increased interest in many applications, including x-ray diffraction [4], electron microscopy [5], wavefront sensing [6,7], and quantitative phase microscopy [8–10].

The TIE is a second-order elliptic partial differential equation that provides quantitative phase using only axially defocused intensity information, allowing for simple and flexible experimental setups. The uniqueness of the TIE solution, however, requires a strictly positive intensity and, more importantly, the precise knowledge of (Dirichlet, Neumann) boundary conditions [11]. To avoid the complexity of obtaining such boundary conditions, the TIE is usually solved under simplified homogeneous boundary conditions or periodic boundary conditions, with use of the fast Fourier transform (FFT)-based TIE solver [12,13]. This method works well when the phase is "flat" at the boundary of the image field of view (FOV) as shown in Fig. 1(a) [14], in which case the energy (intensity) conservation is fulfilled inside the FOV at different image recording locations. Nevertheless, this configuration does not reflect general experimental conditions, and is impractical in many other applications, such as wavefront sensing. For example, as shown in Fig. 1(b), the energy inside the FOV is not conserved, as energy "leak" occurs at the FOV boundary during the recording distance is being changed. In this case, nonhomogeneous boundary conditions are thus required for the correct phase reconstruction based on TIE. The first attempt to solve the TIE under nonhomogeneous boundary conditions has been made by Roddier [6,7] in adaptive optics. Recently, Zuo *et al.* [15] addressed the solution of the TIE in the case of nonhomogeneous Neumann boundary conditions under nonuniform illuminations. By introducing a hard aperture to limit the wavefield under test shown in Fig. 1(c), the energy conservation can be satisfied, and the nonhomogeneous Neumann boundary conditions are directly measured around the aperture edge. In the case of the rectangular aperture, the fast discrete cosine transform (DCT) can be used to solve the TIE effectively and efficiently, which has been well demonstrated in application of microlens characterization [16]. However, one limitation of Zuo's technique is that the fast solution is only available for a rectangular aperture because the DCT only applies to rectangular domains. In practice, it is quite challenging to add an aperture whose shape is exactly a rectangle due to the difficulties in aperture fabrication and system alignment, or the other existing pupils (e.g., reflecting telescopes) obstructing the system aperture to be rectangular. Until now, the solution to the TIE under nonhomogeneous boundary conditions in an arbitrarily shaped region has not been considered explicitly.

In this work, we present a new iterative DCT (iter-DCT) method to solve the TIE with a hard aperture [in the case of Fig. 1(c)], but the aperture shape can be arbitrary. To develop the iter-DCT formalism, we define the complex amplitude of the paraxial beam to be measured as $\sqrt{I(\boldsymbol{r})}\,\exp[ik\phi(\boldsymbol{r})]$, where k is the wave number $2\pi/\lambda$, and $\boldsymbol{r}$ is the position vector representing the 2D spatial coordinates (x, y). $I(\boldsymbol{r})$ is the in-focus image intensity. ∇ is the gradient operator over $\boldsymbol{r}$, which is normal

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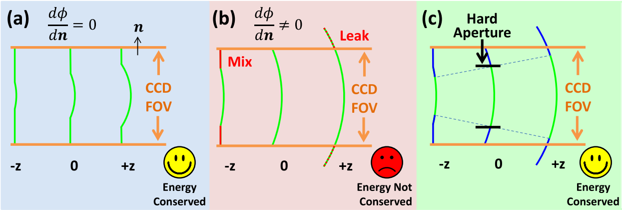

Fig. 1. Energy conservation is required in TIE. (a) Energy is conserved when phase derivatives in the normal directions at boundary edges $d\phi/d\mathbf{n} = 0$. (b) Energy is not conserved when $d\phi/d\mathbf{n} \neq 0$. (c) A hard aperture is added in the optical wavefield to make sure of the energy conservation.

to the beam propagation direction. The TIE is given by [3]

$$-k\frac{\partial I(\boldsymbol{r})}{\partial z} = \nabla \cdot [I(\boldsymbol{r})\nabla\phi(\boldsymbol{r})]. \tag{1}$$

The TIE is conventionally solved under the so-called "Teague's assumption" that the transverse flux $I(\boldsymbol{r})\nabla\phi(\boldsymbol{r})$ is conservative so that can be fully characterized by a scalar potential $\psi(\boldsymbol{r})$ [3]. The substitution $\nabla\psi(\boldsymbol{r}) = I(\boldsymbol{r})\nabla\phi(\boldsymbol{r})$ transforms the TIE into a Poisson equation $\nabla^2\psi(\boldsymbol{r}) = -k\partial I(\boldsymbol{r})/\partial z$, with the solution of the phase taking the following form

$$\phi(\boldsymbol{r}) = -k\nabla^{-2}\nabla \cdot \left[I^{-1}(\boldsymbol{r})\nabla\nabla^{-2}\frac{\partial I(\boldsymbol{r})}{\partial z}\right], \tag{2}$$

where ∇^{-2} is the inverse Laplacian. For simplified homogeneous boundary conditions or periodic boundary conditions defined in a rectangular domain, the inverse Laplacian can be effectively implemented with the FFT [12]. For more general nonhomogeneous Neumann boundary conditions defined on the rectangular domain (with the boundary signal enclosed), the FFT should be replaced by the DCT [15]. It should be noted that the DCT-based TIE solver can also be effectively implemented by combing the FFT-solver with a mirror padding scheme.

Considering the optical field is limited by an arbitrary-shaped aperture, the intensity captured at the in-focus plane $I(\boldsymbol{r})$ will contain a large number of zeros, precluding direct use of Eq. (2) for phase reconstruction ($I(\boldsymbol{r})$ appears in the denominator). Therefore, we "fix" these intensity values beyond the extent of the physical pupil with the average intensity inside, and then the DCT-based TIE solver can be used to get an initial estimation of the phase distribution $\phi_0(\boldsymbol{r})$ (extended over the full support size), as shown in the box in Fig. 2. Since the intensity extrapolation with the average value inside (referring to step D in Fig. 2) is not physically grounded, the $\phi_0(\boldsymbol{r})$ within the aperture is usually an inaccurate solution. Therefore, if we substitute $\phi_0(\boldsymbol{r})$ back to the right hand side of the TIE [Eq. (1)], the resultant intensity derivative on the left-hand side (where we define $J := -k\partial I/\partial z$ for succinctness) will be inconsistent with the real measurement. This inconsistency can be treated as the error signal, which is used as the source term for another round of phase reconstruction. The solution $\Delta\phi_0(\boldsymbol{r})$ is taken as the "correction term," which is added

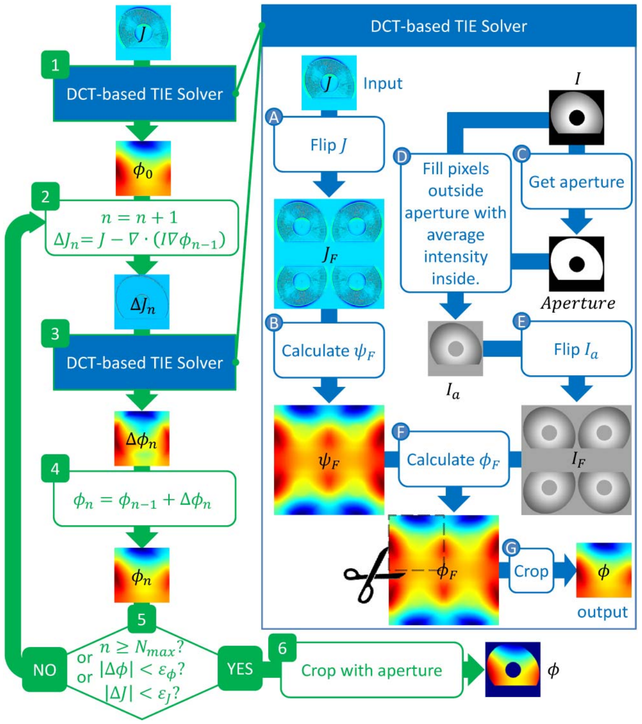

Fig. 2. Iter-DCT-based TIE solver is illustrated for phase retrieval with an arbitrarily shaped hard aperture.

back to $\phi_0(\boldsymbol{r})$ to get an updated phase estimate $\phi_1(\boldsymbol{r})$. The procedure is iteratively repeated until the "stopping criterion" is satisfied. The stopping criterion chosen to assess the convergence is shown in step 5 in Fig. 2. It should be noted that similar iterative algorithms have been proposed to compensate "phase discrepancy" owing to the "Teague's assumption" [17,18], while in this work we adapt it to solve the boundary condition problem instead. By doing so, our approach can directly obtain the "unbiased" solution of the TIE that free from any boundary error and "phase discrepancy," simultaneously.

A simulation is carried out to verify the proposed method. The CCD FOV is $0.512\ \text{mm} \times 0.512\ \text{mm}$ with 256×256 pixels. The wavelength $\lambda = 633$ nm. An irregular aperture is generated to enhance the complexity. The aperture shape is generated with a combination of an ellipse ($x^2 + y^2 - 0.3xy < 0.04096\sqrt{2}$) while its central region is blocked ($x^2 + y^2 > 0.00524288$) and a knife edge ($y < 0.1024\sqrt{2}$) as shown in Fig. 3(a).

The normalized nonuniform intensity is distributed as $I(x, y) = \exp[-(x^2 + y^2)/(2 \times 0.18^2)]$. The in-focus image intensity is captured as Fig. 3(b). The true phase distribution can be theoretically arbitrary and here not purposely set as $\phi(x, y) = 10x^2 - 10y^2 + 0.7x + 2y + 0.82$, which is distributed as shown in Fig. 3(c). Please note only the measurable values inside the aperture are of interest. Two oppositely defocused ($z = \pm 0.5$ mm) images are shown in Figs. 3(d) and 3(e). Once the intensity images are obtained, the intensity derivative $\partial I/\partial z$ can be calculated and shown in Fig. 3(f). The calculated $J := -k\partial I/\partial z$ and the filled intensity shown in Figs. 4(a) and 4(b) are used as the inputs to the DCT-based TIE solver, which results in the initial phase ϕ_0 shown in Fig. 4(c).

After employing the iterative compensations, the standard deviation (STD) of phase error (with piston term ignored) inside aperture is reduced rapidly (see Fig. 5) from the initial STD = 0.095 rad [Fig. 5(a)] down to STD = 0.005 rad [Fig. 5(b)] in 10 iterations. In other words, the accuracy of the retrieved phase is significantly improved (about 19 times better) through the compensations.

The estimated phase distribution in the complete FOV after iterative compensations is shown in Fig. 5(c). Of course, only the values inside the aperture are desired and reliable. The final phase distribution shown in Fig. 5(d) with its corresponding error distributed in Fig. 5(b) indicates the high accuracy of the proposed method.

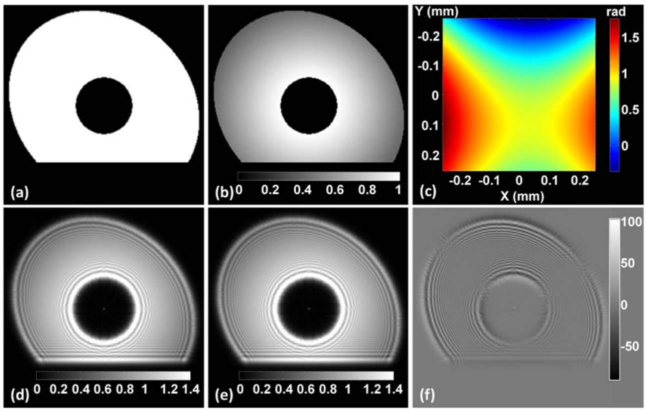

Fig. 3. TIE through a hard aperture, (a) which is in an irregular shape, (b) is simulated with calculated intensity at focus, (c) true phase, (d) calculated intensity at $z = -0.5$ mm and (e) $z = 0.5$ mm, and (f) $\partial I/\partial z$.

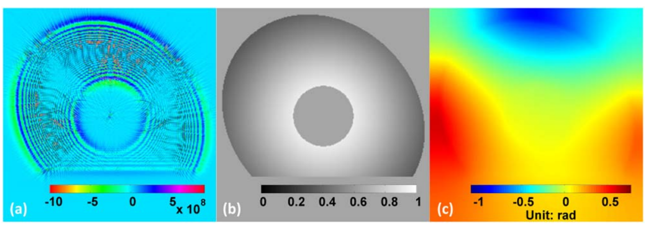

Fig. 4. With the inputs of the calculated J (a) and filled intensity (b), the DCT-based TIE solver can estimate an initial phase (c).

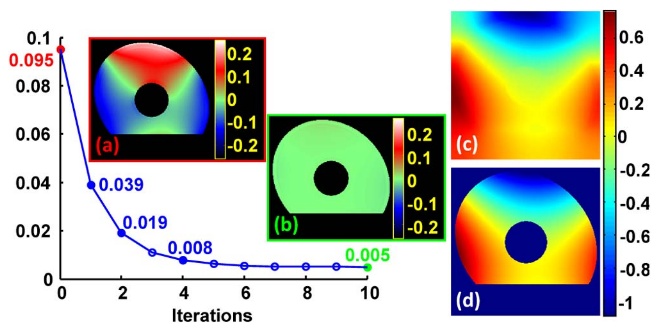

Fig. 5. Proposed iter-DCT method effectively reduces the errors of phase estimation from the initial errors (a) down to the updated ones (b), and the phase in FOV (c) and inside the aperture (d) can be retrieved as results.

In order to demonstrate its feasibility in practice, the proposed method is also tested with a set of real TIE data. As illustrated in Fig. 6, an inverted bright-field microscope (Olympus IX71) attached with an electronically tunable lens-based TIE (TL-TIE) system is used to acquire the intensity images in and out of focus. The pixel size of the CCD (Imaging Source DMK 41AU02 1280 × 960) is 4.65 μm. In our experiment, the wavelength is 550 nm. The specimen is a piece of microlens array. At its image plane, a rectangle-like aperture is introduced. The in-focus image is shown in Fig. 7(a) with its intensity histogram in Fig. 7(b), which indicates it is not difficult to set an intensity threshold to separate the regions in and out of the aperture. By varying the focal length of the tunable lens, the defocused images are sequentially obtained at equivalent defocusing distances of −550 μm in Fig. 7(c) and +550 μm in Fig. 7(d). The intensity derivative $\partial I/\partial z$ is shown in Fig. 7(e).

In order to have a benchmark to compare the accuracy, Zuo's DCT method [15] is implemented by using the data in a rectangular region $\bar{\Omega}$ (within dashed yellow

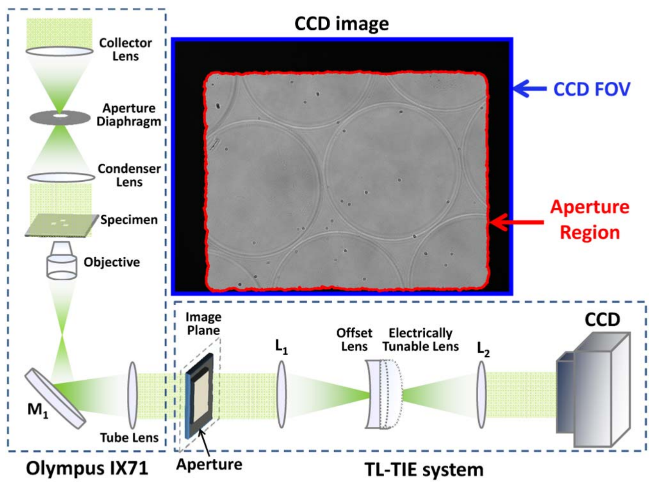

Fig. 6. TIE experiment is implemented by using an inverted bright-field microscope and a tunable lens-based TIE module with placing an aperture at the image plane.

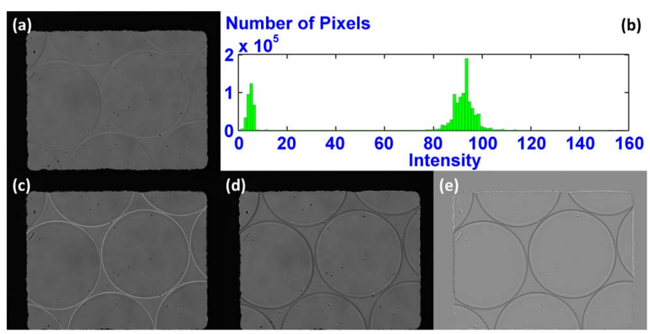

Fig. 7. Experimentally captured intensity at focus (a) with its histogram (b), and the intensity at −550 μm (c) and +550 μm (d) as well as their intensity derivative $\partial I/\partial z$ (e).

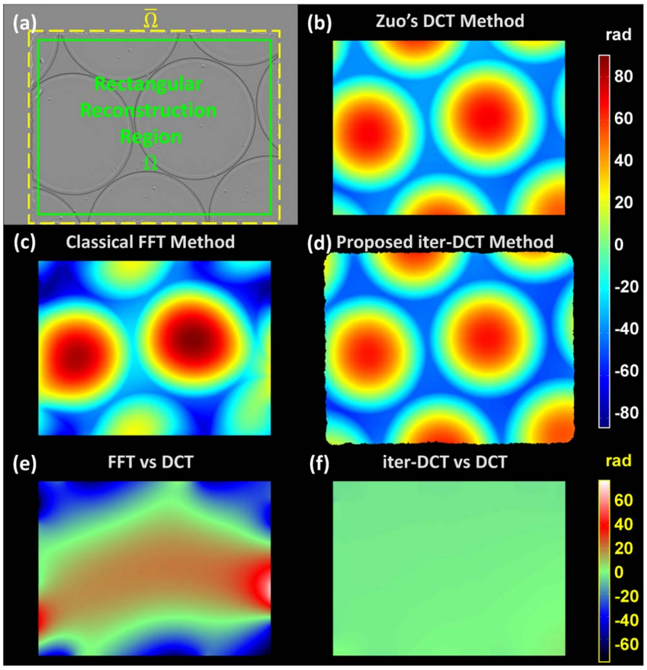

Fig. 8. Zuo's DCT method uses the information in "data region $\bar{\Omega}$" to retrieve phase in reconstruct region Ω (a), and its result (b) is used as a benchmark to judge the results from classical FFT-based TIE solver (c) and the result from the proposed iter-DCT method (d). The phase retrieved with the proposed method is much closer to the DCT result (f) than the FFT one is (e).

lines) including the aperture boundary shown in Fig. 8(a). Due to its characteristics, the phase is only reconstructed within a slightly smaller rectangular region Ω (within solid green lines) instead of the whole $\bar{\Omega}$. The retrieved phase in Fig. 8(b) is going to be a phase benchmark for the following comparison. The classical FFT-based TIE solver is implemented to retrieve the phase within the rectangular region Ω (within solid green lines), whose result is shown in Fig. 8(c). The phase result within the whole irregular aperture shown in Fig. 8(d) is retrieved by the proposed method after 6 iterations. The difference between phase results from classical FFT method and the DCT method is very large (STD $=$ 21.11 rad) as shown in Fig. 8(e), and Fig. 8(f) shows the phase difference between the proposed iter-DCT method and Zuo's DCT one is much smaller (STD $=$ 1.25 rad only). The comparison indicates the proposed method can retrieve more accurate phase distribution than the classical FFT method does under nonhomogeneous Neumann boundary conditions.

Although the proposed phase retrieved is similar to that with the DCT method, it is worthy to note their differences. Theoretically, Zuo's DCT method requires that a rectangular aperture is recorded with its boundaries parallel to the CCD pixel coordinates in order to take DCTs in the selected rectangular regions. Furthermore, the "reconstruction region" is determined based on the defocusing distance and wavelength in use. As a result, it may require some experience to select proper regions for a good result in practice. On the other hand, the method proposed in this work handles apertures in arbitrary shapes and does not care about the relations between aperture edges and image coordinates. Moreover, the proposed method treats input images as a whole piece of data without cutting any regions in advance, and consequently it is pretty straightforward to use in practice. When both methods are applicable, it is not easy to say which one is more accurate as many factors (e.g., noise, region selection) can influence the accuracy.

In this work, an iter-DCT-based TIE solver is proposed for phase retrieval under nonuniform illuminations and nonhomogeneous boundary conditions in an arbitrarily shaped region. In hardware, the added aperture can be in an arbitrary shape, which results in a low requirement on aperture fabrication and alignment. In data processing, the procedure is extremely automatic and easy to use. These features of the proposed method significantly enhance the flexibility of TIE measurement with hard aperture in real applications.

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References

1. L. Huang, Q. Kemao, B. Pan, and A. K. Asundi, Opt. Lasers Eng. **48**, 141 (2010).
2. J. R. Fienup, Appl. Opt. **21**, 2758 (1982).
3. M. Reed Teague, J. Opt. Soc. Am. **73**, 1434 (1983).
4. K. A. Nugent, Adv. Phys. **59**, 1 (2009).
5. S. Bajt, A. Barty, K. A. Nugent, M. McCartney, M. Wall, and D. Paganin, Ultramicroscopy **83**, 67 (2000).
6. F. Roddier, Appl. Opt. **29**, 1402 (1990).
7. F. Roddier and C. Roddier, Appl. Opt. **30**, 1325 (1991).
8. A. Barty, K. A. Nugent, D. Paganin, and A. Roberts, Opt. Lett. **23**, 817 (1998).
9. C. Zuo, Q. Chen, W. Qu, and A. Asundi, Opt. Lett. **38**, 3538 (2013).
10. L. Waller, Y. Luo, S. Y. Yang, and G. Barbastathis, Opt. Lett. **35**, 2961 (2010).
11. T. E. Gureyev, A. Roberts, and K. A. Nugent, J. Opt. Soc. Am. A **12**, 1942 (1995).
12. D. Paganin and K. A. Nugent, Phys. Rev. Lett. **80**, 2586 (1998).
13. T. E. Gureyev and K. A. Nugent, Opt. Commun. **133**, 339 (1997).
14. J. Martinez-Carranza, K. Falaggis, T. Kozacki, and M. Kujawinska, Proc. SPIE **8789**, 87890N (2013)
15. C. Zuo, Q. Chen, and A. Asundi, Opt. Express **22**, 9220 (2014).
16. C. Zuo, Q. Chen, H. Li, W. Qu, and A. Asundi, Opt. Express **22**, 18310 (2014).
17. C. Zuo, Q. Chen, L. Huang, and A. Asundi, Opt. Express **22**, 17172 (2014).
18. A. Shanker, M. Sczyrba, B. Connolly, F. Kalk, A. Neureuther, and L. Waller, Proc. SPIE **9052**, 90521D (2014).