Phase retrieval with iterative compensation based on the transport-of-intensity equation

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A transport-of-intensity equation (TIE) as a quantitative method for phase retrieval should be solved under the appropriate boundary conditions. Thus, to improve the convenience of operation, we put an arbitrarily shaped aperture into the optical wave-field which can make the Neumann boundary conditions directly measured and satisfy the energy conservation. With the nonhomogeneous boundary conditions, an iterative compensation method is proposed which uses a maximum in-focus intensity value instead of the true distribution to avoid zero and near zero values. Comparing to the existing compensation methods, the proposed mechanism has no need to obtain the exact boundary position and can sharply reduce the iteration time. In addition, it can effectively avoid phase discrepancy which originates from the Teague’s assumption. Simulations and experiments with the arbitrary aperture shapes and nonuniform intensity distribution have verified the effectiveness and accuracy of the proposed method, which will make TIE technique more flexible and less time-consuming for phase retrieval in practice.

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Phase is a central problem permeating many areas of physics and optics, e.g., electron and x-ray microscopy [1], crystallography [2], diffraction tomography [3], but unfortunately it is not accessible directly. Several methods for phase reconstruction from the relatively easy-measured intensity are being sought, which can be categorized into two main streams, namely qualitative phase contrast imaging [4, 5] and quantitative phase imaging (QPI) [6–10]. However, the first group of phase imaging methods only provide the qualitative phase images of sample, and it is difficult to process the phase image for quantitative data interpretation, such as the refractive index, optical thickness, and the topology of the specimen. Over the past decade, there has appeared an increasing demand for quantitative phase imaging, and thus QPI as an effective approach to recover the phase of transparent/unlabeled samples attracts more attention. Comparing to some interference approaches, for example, the conventional off-axis digital holographic microscopy (DHM) [8–10] providing the total phase delay of sample by the spatial modulation of homogeneous/heterogeneous refractive index within the sample, the non-interferometric and deterministic phase retrieval algorithms like transport-of-intensity equation (TIE) can avoid speckle noise and external interferometric reference beam, reduce costs of setups and dependence on the environment, and directly obtain the unwrapping phase information.

Although the TIE is a second-order elliptic partial differential equation that provides quantitative phase using only axially defocused intensity information, the uniqueness of the TIE solution requires a strictly positive intensity, and more importantly, the precise knowledge of (Dirichlet, Neumann) boundary conditions [7, 11]. Thus, soft-edged intensity profile, such that the intensity distribution is non-zero inside the domain but drops to zero at the boundary (generating the simplified homogeneous boundary or periodic boundary conditions), is employed to avoid the complexity of obtaining boundary conditions and then the TIE is usually solved with use of the fast Fourier transform (FFT) [12, 13] or Zernike polynomial expansion [12, 14]. Nevertheless, in many applications, such soft-edged intensity acquisition is impractical, and many researches addressed the solutions of the TIE in the case of nonhomogeneous Neumann boundary conditions under nonuniform illuminations which reflects general experimental conditions [6, 7, 15]. Among these methods, introducing a hard aperture to limit the wave-field to satisfy the energy conservation and directly measure the nonhomogeneous Neumann boundary conditions around the aperture edge is more practical, especially the arbitrary shaped apertures [7]. The recent iterative discrete cosine transforms (iter-DCT) method [7] has succeeded in phase retrieval under nonuniform illumination and nonhomogeneous boundary conditions, but it needs to obtain the exact boundary position and the iteration
time will fold increase due to the multiple use of the discrete cosine transforms based solvers.

In this work, to solve the above-mentioned problems including boundary conditions, phase discrepancy, and time-consuming, we present a new robust iterative FFT (robust-iter-FFT) method to solve the TIE with a hard apertures, which can have arbitrary shape. To develop the robust-iter-FFT formalism, firstly the given TIE [16] is:

\[- k \frac{\partial I(r)}{\partial z} = \nabla \cdot [I(r) \nabla \phi(r)] \quad (1)\]

where \( I(r) \) is the in-focus image intensity, \( r \) is the position vector representing the 2D spatial coordinates \((x, y)\), \( \phi(r) \) is the phase information, \( k \) is the wave number \(2\pi/\lambda\), \( \lambda \) is the incident wavelength. To acquire the phase information \( \phi(r) \), the TIE is solved under the so-called "Teague’s assumption” that the transverse flux \( I(r) \nabla \phi(r) \) is conservative so that can be fully characterized by a scalar potential in traditional proposed methods [16]. Thus, the phase information can be obtained by

\[
\phi(r) = -k \nabla^{-2} \left\{ \frac{1}{I(r)} \nabla^{-2} \left[ \frac{\partial I(r)}{\partial z} \right] \right\} \quad (2)
\]

However, Teague’s assumption will result in the phase discrepancy, which neglects the curl term according to the Helmholtz decomposition theorem to make a silent hypothesis that the transverse flux is irrotational [17]. Moreover, in the actual situation, considering that the optical field is limited by an arbitrary shaped aperture, the intensity captured at the in-focus plane \( I(r) \) will contain many values close to zero, precluding direct use of Eq. 2 for phase reconstruction where \( I(r) \) appears in the denominator. Fortunately, we can find that when intensity is uniform, the denominator in Eq. 2 can effectively avoid the above-mentioned zero values and Teague’s assumption will be unnecessary. Thus, we consider using the maximum value of the in-focus image intensity \( I_{\text{max}} \) as the uniform intensity, and then the solution of the phase will take the following form:

\[
\phi(r) = -k \frac{\nabla^{-2}}{I_{\text{max}}} \left[ \frac{\partial I(r)}{\partial z} \right] \quad (3)
\]

where the inverse Laplace operator \( \nabla^{-2} \) can be obtained by using a pair of Fourier transform. Eq. 3 can be rewritten as:

\[
\phi(r) = F^{-1} \left\{ \frac{8\pi^3 |u|^2}{A_{\text{max}}} F \left[ \frac{\partial I(r)}{\partial z} \right] \right\} \quad (4)
\]

where \( u \) is the 2D coordinate in frequency domain, \( F \) and \( F^{-1} \) respectively represents Fourier transform and inverse Fourier transform. Because \( I_{\text{max}} \) is not the true in-focus intensity, the phase calculated by Eq. 4 will generates distortion, and then a compensation mechanism will be introduced to acquire the exact solution, as shown in Fig. 1. The proof of convergence of iterative process can be found in Supplementary Information.

**Step1: Calculate intensity derivative.** Capture the images on different planes and calculate the intensity derivative \( \Delta I_0 = \bar{J}_0 = \frac{\partial I(0)}{\partial z} \). The initial estimation of the phase distribution is \( \phi_0 = 0 \) for succinctness.

**Step2: Calculate artificial phase discrepancy.** The intensity derivative discrepancy \( \Delta J_{n-1} \) will be used to calculate the artificial phase discrepancy \( \phi_{n-1} \) based on Eqs. (3,4), where \( n \) represents the number of iteration.

**Step3: Calculate artificial intensity discrepancy.** \( \phi_{n-1} \) will be substituted into Eq. 1 to calculate the actual intensity derivative \( J_n \) corresponding to the artificial phase discrepancy \( \phi_{n-1} \).

**Step4:** Calculate intensity derivative discrepancy. \( J_n \) calculated in Step 3 contains information distortion essentially arising from the uniform assumption. Then the intensity derivative discrepancy between \( \Delta J_{n-1} \) and \( J_n \) will be generated for the next artificial phase discrepancy calculation.

**Step5:** Calculate phase. Phase obtained in last iteration have artifacts and the output in Step 2 will be used for compensation.

**Step6:** Determine whether the loop terminates. When the maximum iterations \( N_{\text{max}} \) is reached or the artificial phase/intensity derivative discrepancy is small enough, the compensation loop will stop, otherwise \( \phi_{n-1} \) and \( J_n \) will be used in the next iteration for phase compensation.

It should be noted that similar iterative algorithms have been proposed to compensate phase discrepancy owing to the Teague’s assumption [6, 17]. In this work, the new approach can directly obtain the solution of the TIE that free from boundary error and essentially avoiding phase discrepancy. In addition, the iteration speed will be dramatically accelerated, because this method sharply reduce the number of Fourier transforms pairs.

A simulation is carried out to verify the reliability and effectiveness of the proposed method. The field-of-view (FOV) of the camera is \( 0.512 \times 0.512 \text{mm}^2 \) with \( 2\mu \text{m} \) pixel size. The irregular apertures respectively are an circle and a combination of a knife edge and an ellipse blocked by a circle in central region as shown in Figs. 2(a1,b1). The in-focus intensity images as illustrated in Figs. 2(a2,b2) are suggested to be the Gaussian distribution. The phase distribution here is assumed to be \( \phi(r) = 10r_x^2 - 10r_y^2 - 0.7r_x + 2r_y + 0.82 \), as shown in Figs. 2(a3,b3). It should be noted that only the measurable values inside the apertures are of interest. Two oppositely defocused images \( z = \pm 1 \mu \text{m} \) are obtained to calculate the intensity derivative \( \partial I(r)/\partial z \) [Figs. 2(a4,b4)], which is used as the input to the TIE solver. The final reconstructed phase distribution and phase discrepancy are separately shown in Figs. 2(a5,b5,a6,b6).

In order to verify that the proposed robust-iter-FFT method can effectively reduce the iteration time, we compare this method with Iter-DCT method[7]. The simulation conditions in
The simulation results of the iterative compensation method with hard apertures. (a1,b1) The different shapes of hard apertures. (a2,b2) The calculated intensity on focus plane. (a3,b3) The true phase. (a4,b4) The intensity derivative \( \Delta I_0 = I_0 = \partial I / \partial z \). (a5,b5) The retrieved phase inside the aperture. (a6,b6) The errors inside the aperture.

Figs. 2(b1-b6) are used for both methods. As the number of iterations increases, the root mean squared error (RMSE) of the reconstructed results with the reported method decreases rapidly, and the RMSE value tends to zero at about 40 iterations as shown in Fig 3 (the orange solid line). Although the RMSE value of the new method is larger than that of the iter-DCT method before 40 iterations, the time-consuming of the new method with the same number of iterations is far below that of the iter-DCT method (the dotted line in Fig 3). The inserted figure more intuitively shows the time-consuming curves of RMSE values, and the RMSE values of the new proposed method decreases dramatically as time increasing, from the initial RMSE 0.2709 down to 0.0027 in 0.6850 seconds in Matlab with a personal computer using an Intel i7-7700HQ CPU (no GPU).

In addition, to demonstrate the feasibility of the robust-iter-FFT method in practice, it is also tested with a set of real TIE data. As illustrated in Fig. 4, an inverted bright-field microscope (Olympus IX83) attached with 4f imaging system is used to acquire the intensity images in and out of focus by slightly mechanical moving the camera. The pixel size of the camera is 96.283s in Matlab when the number of iterations is 20. By contrast, the new method can dramatically reduce the consuming time to 8.287s.

![Fig. 2](image2.png)

**Fig. 2.** The simulation results of the iterative compensation method with hard apertures. (a1,b1) The different shapes of hard apertures. (a2,b2) The calculated intensity on focus plane. (a3,b3) The true phase. (a4,b4) The intensity derivative \( \Delta I_0 = I_0 = \partial I / \partial z \). (a5,b5) The retrieved phase inside the aperture. (a6,b6) The errors inside the aperture.

![Fig. 3](image3.png)

**Fig. 3.** The curve (solid line) of the iteration number and the root mean squared error (RMSE). The curve (dotted line) of the iteration number and accumulated time. The inserted figure is the curve of the iteration time (50 iterations) and RMSE.

![Fig. 4](image4.png)

**Fig. 4.** The experimental setup is implemented by using an inverted bright-field microscope and a 4f system-based TIE module with an aperture at the image plane.

![Fig. 5](image5.png)

**Fig. 5.** (a) The initial intensity derivative \( \Delta I_0 = I_0 = \partial I / \partial z \). (b) The result with the classical FFT-based TIE solver. (c-d) The reconstructed phase distribution separately based on the iter-DCT and robust-iter-FFT methods.
In addition, in order to verify the applicability of this new method under irregular boundary conditions, we carried out experiments by changing the rectangle boundary into an octagonal one. Fig. 6(a) is the original captured image showing that parts of the sample are at the boundary. According to the histogram, the aperture can be obtained as shown in Fig. 6(c), and the result [Fig. 6(d)] can be recovered based on the FFT-based TIE solver when the zero-value region is filled with a small value. The retrieved phase based on the proposed method is shown in Fig. 6(e), and comparing to the result in Fig. 6(d), the information on the boundary can be recovered more accurately. More specifically, when the same lens is selected, the cross-sectional comparison of the phase results is shown in Fig. 6(f). From Fig. 6(f), it can be directly concluded that the lateral length of a single lens is about 249.55 μm and the phase is about 150 rad. Theoretically, the horizontal length of each lens (SUSS, Nr.18-00035) is 250 μm and the phase is in the range of 149 ~ 166 rad with the illumination at 550 nm wavelength. Thus, the reconstruction is consistent with the theoretical value.

The new method can also be used for phase imaging of unstained cells, as shown in Fig. 7. The boundary position is obtained only by simple thresholds. Comparing to the traditional solver [Fig. 7(c)], under the nonhomogeneous Neumann boundary conditions, the results based on the new method can provide more smooth background, reveal more details, and enhance contrast especially the membranes of the cells.

In this work, a robust-iter-FFT-based TIE solver is proposed for phase retrieval under nonuniform illuminations and nonhomogeneous boundary conditions. Comparing to the traditional structure, the new one only needs to add an arbitrary shape with low requirement in fabrication and alignment. And most importantly, after obtaining the data, the new data processing method uses the maximum in-focus intensity value to avoid the in-focus intensity containing a large number of zeros, sharply accelerate the iterative process, and essentially eliminate the phase discrepancy resulting from the Teague’s assumption. These characteristics of the reported method will significantly benefit for the TIE measurement with hard aperture in real applications.

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