Supplementary Information: On a universal solution to the transport-of-intensity equation

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This document provides supplementary information for "Phase retrieval with iterative compensation based on the transport-of-intensity equation". This supplementary information is mainly about the proof of convergence of the proposed method in this paper.

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A. The description for the robust iteration method

The transport-of-intensity equation is

$$-k\frac{\partial I(\mathbf{r})}{\partial z} = \nabla \cdot [I(\mathbf{r}) \nabla \phi(\mathbf{r})], \tag{S1}$$

where $I(\mathbf{r})$ is the in-focus image intensity, $\mathbf{r}$ is the position vector representing the 2D spatial coordinates (x, y), $\phi(\mathbf{r})$ is the phase information, k is the wave number $2\pi/\lambda$, λ is the incident wave-length. Thus, the equation can be considered as

$$\nabla \cdot [I(\mathbf{r}) \nabla \phi(\mathbf{r})] = -kJ_0 \tag{S2}$$

with some Neumann boundary condition $\nabla\phi \cdot \gamma = \beta$ on a square Ω. Here β is a known function defined on $\partial\Omega$, γ is the outer unit normal vector, $-kJ_0 = -k\partial I(\mathbf{r})/\partial z$ is a constant.

The method can be noted as the following:

Step1: Let φ_0 satisfies the equation:

$$\nabla \cdot (I_{\max} \nabla \varphi_0) = -kJ_0 \tag{S3}$$

with the Neumann boundary condition $\nabla\phi_0 \cdot \gamma = \beta$. Here $I_{\max}$ means the maximum value of I on Ω. Then ϕ_0 can be calculated.

Step2: Suppose that φ_n has been solved, the let φ_{n+1} satisfies the equation

$$\nabla \cdot (I_{\max} \nabla \varphi_{n+1}) = \nabla \cdot ((I_{\max} - I) \nabla \varphi_n) \tag{S4}$$

with homogeneous Neumann boundary condition, i.e. $\nabla\varphi_{n+1} \cdot \gamma = 0$. Then calculate ϕ_{n+1} by the same numerical algorithm. Then we can calculate a sequence $\{\varphi_n\}_{n=0}^{\infty}$. Here Eq. S4 is equivalent to **Step *Calculate intensity derivative discrepancy*** in the original paper ($\Delta J_n = \Delta J_{n-1} - J_n$).

Step3: When $\phi = \sum\limits_{n=0}^{\infty} \varphi_n$, we hope ϕ is the solution of Eq. S2, and thus two conditions must be satisfied.

1) The series $\{\varphi_n\}_{n=0}^{\infty}$ is convergent.
2) The ϕ can satisfies Eq. S2.

Section B to **Section F** are derived under the following assumptions:

1) The function $I(\mathbf{r})$ belongs to the Lipschitz spaces.
2) For any $\mathbf{r} \in \Omega$, $I(\mathbf{r}) > 0$.

B. $W^{1,2}$ estimations for φ_n

$W^{1,2}$ represents one sobolev space[1], and in this space, the square of the first derivative of all functions is integrable. When $n > 1$, Eq. S4 can be noted as

$$\iint_\Omega \nabla^2 \varphi_{n+1}\varphi_{n+1}dxdy = \iint_\Omega \nabla\left(\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right)\varphi_{n+1}dxdy. \tag{S5}$$

Then according to the Hölder inequality, Eq. S5 can be rewritten as

$$\iint_\Omega |\nabla\varphi_{n+1}|^2 dxdy = \iint_\Omega \left(\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right)\nabla\varphi_{n+1}dxdy \leqslant \left(\iint_\Omega \left|\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right|^2 dxdy\right)^{1/2}\left(\iint_\Omega |\nabla\varphi_{n+1}|^2 dxdy\right)^{1/2}, \tag{S6}$$

which means that

$$\left(\iint_\Omega |\nabla\varphi_{n+1}|^2 dxdy\right)^{1/2} \leqslant \left(\iint_\Omega \left|\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right|^2 dxdy\right)^{1/2} \leqslant \left\|\frac{I_{\max}-I}{I_{\max}}\right\|_{L^\infty(\Omega)}\left(\iint_\Omega |\nabla\varphi_n|^2 dxdy\right)^{1/2}. \tag{S7}$$

Then by the induction, we know that

$$\|\varphi_{n+1}\|_{W^{1,2}(\Omega)} \leqslant \left(\left\|\frac{I_{\max}-I}{I_{\max}}\right\|_{L^\infty(\Omega)}\right)^n \|\varphi_1\|_{W^{1,2}(\Omega)}. \tag{S8}$$

Thus, $\phi = \sum\limits_{n=0}^{\infty}\varphi_n$ belongs to $W^{1,2}(\Omega)$, provided that φ_0 and φ_1 also belong to $W^{1,2}(\Omega)$. According to the Sobolev embedding theorem [2, 3], when $W^{p,q}(\Omega)$ needs to be embedded in $L^\infty(\Omega)$, the product of p and q needs to be larger than the space dimension (here the dimension is 2). Thus, $W^{1,2}$ cannot be embedded in $L^\infty(\Omega)$.

C. $W^{2,2}$ estimations for φ_n

From Eq. S4, we also have the following equation for $h > 0$ small enough

$$\iint_\Omega \nabla\varphi_{n+1}D_x^{-h}\nabla D_x^h\varphi_{n+1}dxdy = \iint_\Omega \frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n D_x^{-h}\nabla D_x^h\varphi_{n+1}dxdy. \tag{S9}$$

Here $D_x^h\varphi_{n+1}(x,y) = [\varphi_{n+1}(x+h,y)-\varphi_{n+1}(x,y)]/h$. We extend φ_{n+1} to a bigger domain $\Omega' = \Omega\cup[-h_0,0]\times[0,1]\cup[1,1+h_0]\times[0,1]\cup[0,1]\times[-h_0,0]\cup[0,1]\times[1,1+h_0]$ where $h_0 > 0$ is small enough. For the left hand side, we have that

$$\iint_\Omega \nabla\varphi_{n+1}D_x^{-h}\nabla D_x^h\varphi_{n+1}dxdy = -\iint_\Omega D_x^h\nabla\varphi_{n+1}\nabla D_x^h\varphi_{n+1}dxdy + J_1 + J_2, \tag{S10}$$

where

$$J_1 = -\frac{1}{h}\iint_{[-h_0,0]\times[0,1]} \nabla\varphi_{n+1}(x+h,y)\nabla D_x^h\varphi_{n+1}(x,y)\,dxdy,$$

and

$$J_2 = \frac{1}{h}\iint_{[1-h_0,0]\times[0,1]} \nabla\varphi_{n+1}(x+h,y)\nabla D_x^h\varphi_{n+1}(x,y)\,dxdy.$$

By the similar arguments, for the right hand side, we also have that

$$\iint_\Omega \frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n D_n^{-h}\nabla D_n^h\varphi_{n+1}dxdy = -\iint_\Omega D_n^h\left(\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right)\nabla D_n^h\varphi_{n+1}dxdy + J_3 + J_4, \tag{S11}$$

where

$$J_3 = -\frac{1}{h}\iint_{[-h_0,0]\times[0,1]} \frac{I_{\max}-I(x+h,y)}{I_{\max}}\nabla\varphi_{n+1}(x+h,y)\nabla D_x^h\varphi_{n+1}(x,y)\,dxdy,$$

and

$$J_4 = \frac{1}{h}\iint_{[1-h_0,0]\times[0,1]} \frac{I_{\max}-I(x+h,y)}{I_{\max}}\nabla\varphi_{n+1}(x+h,y)\nabla D_x^h\varphi_{n+1}(x,y)\,dxdy.$$

Let h tends to $0+$. Then J_i tends to 0 for each $i = 1,2,3,4$. Thus based on Hölder inequality,

$$\begin{aligned}\iint_\Omega |D_x\nabla\varphi_{n+1}|^2 dxdy &= \iint_\Omega D_x\left(\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right)D_x\nabla\varphi_{n+1}dxdy \\ &\leqslant \left(\iint_\Omega \left|D_x\left(\frac{I_{\max}-I}{I_{\max}}\nabla\varphi_n\right)\right|^2 dxdy\right)^{1/2}\left(\iint_\Omega |D_x\nabla\varphi_{n+1}|^2 dxdy\right)^{1/2}.\end{aligned} \tag{S12}$$

This means that for any $\varepsilon > 0$,

$$\begin{aligned}\iint_\Omega |D_x \nabla \varphi_{n+1}|^2 dxdy &\leqslant \iint_\Omega \left| \frac{I_{\max} - I}{I_{\max}} D_x \nabla \varphi_n - \frac{\nabla I}{I_{\max}} \varphi_n \right|^2 dxdy \\ &\leqslant (1+\varepsilon) \iint_\Omega \left| \frac{I_{\max} - I}{I_{\max}} D_x \nabla \varphi_n \right|^2 dxdy + \iint_\Omega \left(1 + \frac{1}{\varepsilon}\right) \left| \frac{\nabla I}{I_{\max}} \varphi_n \right|^2 dxdy \\ &\leqslant (1+\varepsilon) \left\| \frac{I_{\max} - I}{I_{\max}} \right\|^2_{L^\infty(\Omega)} \iint_\Omega |D_x \nabla \varphi_n|^2 dxdy + \left(1 + \frac{1}{\varepsilon}\right) \left[\frac{Lip(\varphi)}{I_{\max}} \right]^2 \iint_\Omega |\nabla \varphi_n|^2 dxdy.\end{aligned} \tag{S13}$$

$Lip\,(\varphi)$ represents the maximum of ∇I in the Lipschitz spaces. Then from the induction and the conclusion in **Section B**, we can obtain

$$\begin{aligned}\iint_\Omega |D_x \nabla \varphi_{n+1}|^2 dxdy &\leqslant \left[(1+\varepsilon) \left\| \frac{I_{\max} - I}{I_{\max}} \right\|^2_{L^\infty(\Omega)} \right]^n \iint_\Omega |D_x \nabla \varphi_1|^2 dxdy \\ &\quad + \left(1 + \frac{1}{\varepsilon}\right) \left[\frac{Lip(\varphi)}{I_{\max}} \right]^2 n(1+\varepsilon)^{n-1} \left\| \frac{I_{\max} - I}{I_{\max}} \right\|^{2n-2}_{L^\infty(\Omega)} \iint_\Omega |\nabla \varphi_1|^2 dxdy.\end{aligned} \tag{S14}$$

Here we also used the assumption that $I\,(x,y)$ belongs to the Lipschitz spaces. By the same arguments, we also obtain that

$$\begin{aligned}\iint_\Omega |D_y \nabla \varphi_{n+1}|^2 dxdy &\leqslant \left[(1+\varepsilon) \left\| \frac{I_{\max} - I}{I_{\max}} \right\|^2_{L^\infty(\Omega)} \right]^n \iint_\Omega |D_y \nabla \varphi_1|^2 dxdy \\ &\quad + \left(1 + \frac{1}{\varepsilon}\right) \left[\frac{Lip(\varphi)}{I_{\max}} \right]^2 n(1+\varepsilon)^{n-1} \left\| \frac{I_{\max} - I}{I_{\max}} \right\|^{2n-2}_{L^\infty(\Omega)} \iint_\Omega |\nabla \varphi_1|^2 dxdy.\end{aligned} \tag{S15}$$

Thus,

$$\|\varphi_n\|_{W^{2,2}(\Omega)} \leqslant \sqrt{1 + \frac{1}{\varepsilon}} \frac{Lip(\varphi)}{I_{\max}} \left[\sqrt{(1+\varepsilon)} \left\| \frac{I_{\max} - I}{I_{\max}} \right\|_{L^\infty(\Omega)} \right]^{n-2} n \|\varphi_1\|_{W^{2,2}(\Omega)}. \tag{S16}$$

D. $W^{2,2}$ estimates for φ_0 and φ_1

The global $W^{2,2}$ estimates for φ_0 and φ_1 are standard. We can get that

$$\|\varphi_0\|_{W^{2,2}(\Omega)}, \|\varphi_1\|_{W^{2,2}(\Omega)} \leqslant C', \tag{S17}$$

where C' is a positive constant depending on I, β and $-kJ_0$. We omit the proof.

E. The convergence

Note that

$$\begin{aligned}\|\phi\|_{W^{2,2}(\Omega)} &\leqslant \left\| \sum_{k=0}^{\infty} \varphi_n \right\|_{W^{2,2}(\Omega)} \leqslant \sum_{k=0}^{\infty} \|\varphi_n\|_{W^{2,2}(\Omega)} \leqslant \|\varphi_0\|_{W^{2,2}(\Omega)} + \|\varphi_1\|_{W^{2,2}(\Omega)} + \sum_{n=2}^{\infty} \|\varphi_n\|_{W^{2,2}(\Omega)} \\ &\leqslant \|\varphi_0\|_{W^{2,2}(\Omega)} + \|\varphi_1\|_{W^{2,2}(\Omega)} + \|\varphi_1\|_{W^{2,2}(\Omega)} \sqrt{1 + \frac{1}{\varepsilon}} \frac{Lip(\varphi)}{I_{\max}} \sum_{n=2}^{\infty} n \left(\sqrt{1+\varepsilon} \left\| \frac{I_{\max} - I}{I_{\max}} \right\|_{W^{2,2}(\Omega)} \right)^{n-2}.\end{aligned} \tag{S18}$$

By choosing ε small enough such that $\sqrt{1+\varepsilon} \|(I_{\max} - I)\,/\,I_{\max}\|_{W^{2,2}(\Omega)} < 1$, the above series is convergent. This means that ϕ belongs to $W^{2,2}\,(\Omega)$. From the Sobolev's Embedding Theorem[2, 3], ϕ also belongs to $L^\infty\,(\Omega)$ space, which means that ϕ is bounded.

Now we only need to show that ϕ is the solution of the Eq. S1. In fact, because of the convergence of the series $\sum_{n=0}^{\infty} \varphi_n$, for any $\psi \in W^{1,2}\,(\Omega)$, based on Eqs. (S2,S3),

$$\begin{aligned}&\iint_\Omega I \nabla \phi \nabla \psi dxdy = \iint_\Omega I \nabla \left(\sum_{n=0}^{\infty} \varphi_n \right) \nabla \psi dxdy = \iint_\Omega I \sum_{n=0}^{\infty} \nabla \varphi_n \nabla \psi dxdy \\ &= \sum_{n=0}^{\infty} \iint_\Omega I \nabla \varphi_n \nabla \psi dxdy = \sum_{n=0}^{\infty} \iint_\Omega I_{\max} \nabla \varphi_n \nabla \psi dxdy - \sum_{n=0}^{\infty} \iint_\Omega (I_{\max} - I) \nabla \varphi_n \nabla \psi dxdy \\ &= \iint_\Omega I_{\max} \nabla \varphi_0 \nabla \psi dxdy + \sum_{n=1}^{\infty} \iint_\Omega [I_{\max} \nabla \varphi_n - (I_{\max} - I) \nabla \varphi_{n-1}] \nabla \psi dxdy \\ &= -\iint_\Omega kJ_0 \psi dxdy + \sum_{n=1}^{\infty} 0 = -\iint_\Omega kJ_0 \psi dxdy .\end{aligned} \tag{S19}$$

From the arbitrariness of ψ in $W^{1,2}(\Omega)$, we know that ϕ satisfies the Eq. S2 and on $\partial\Omega$ we can obtain

$$\nabla\phi \cdot \nu = \left(\nabla \sum_{n=0}^{\infty} \varphi_n\right) \cdot \nu = \sum_{n=0}^{\infty} \nabla\varphi_n \cdot \nu = \beta. \tag{S20}$$

This means that ϕ satisfies the Neumann boundary condition. From the above arguments, we know that ϕ is the solution of Eq. S2 with the boundary condition $\nabla\phi \cdot \nu = \beta$.

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