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A practical way to resolve ambiguities in wavefront reconstructions by the transport of intensity equation

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ABSTRACT

The transport of intensity equation (TIE) provides a very straight forward way to computationally reconstruct wavefronts from measurements of the intensity and the derivative of this intensity along the optical axis of the system. However, solving the TIE requires knowledge of boundary conditions which cannot easily be obtained experimentally. The solution one obtains is therefore not guaranteed to be accurate. In addition, noise and systematic measurement errors can very easily lead to low-frequency artefacts. In this paper we solve the TIE by the finite element method (FEM). The flexibility of this approach allows us to define additional boundary conditions (e.g. a flat phase in areas where there is no object) that lead to a correct solution of the TIE, even in the presence of noise.

1. Introduction

Coherent elastic scattering of light, electrons, or neutrons by matter is effectively described by the modulation and propagation of complex-valued wave functions. Within the phase object approximation, the phase of a wave that has passed through an object is proportional to the time it has taken to transmit the object at that position. This time is proportional to the object's thickness and effective refractive index for the probing type of radiation, i.e. the optical refractive index for light, the electrostatic potential for electrons, and the magnetic field for neutrons. Since this phase information is lost during conventional detection, retrieving the phase of the transmitted wave function is of great importance in fields such as light and electron microscopy, neutron radiography [1], hard X-ray imaging [2], and X-ray computed tomography [3]. Different acquisition methods and computational reconstruction algorithms based on intensity measurements have been developed.

Interferometric techniques which retrieve phase information by transforming phase contrast to intensity variations are well-established methods and are routinely applied in several fields of science (e.g. off-axis holography, Mach–Zehnder interferometer). Interferometric methods rely typically on phase difference between two (partial) waves. In the transmission geometry one of these travels through the object (the object wave) and experiences a distortion of its wave front, while the other is an undistorted reference wave. Interference of the reference wave with the modified object wave results in the formation of fringes in the image plane from which relative phase information can be deduced. However, technical complexity, the need for highly coherent illumination and stability are some of the major obstacles [4].

Non-interferometric methods, such as wave front reconstruction from a series of defocused images on the basis of the Transport of Intensity Equation (TIE) [5], are a viable alternative where interferometric techniques are not practical for the above mentioned reasons. TIE-based methods make use of changes in the intensity of the detected images when propagating a given wave and have gained tremendous attention in the past decades owing to their uncomplicated mathematical formulation and a relatively simple experimental procedure. The TIE is a partial differential equation which relates a modified Laplacian of the phase of the wave to the variation of irradiance along the optical axis. The measurement of the variation of irradiance along the optical axis is typically done by a finite difference approach, i.e. it is approximated by the difference of intensity measurements recorded at different planes of focus, normalized by the difference in defocus. This makes the TIE typically only valid for measurements characterized by small Fresnel numbers [6]. It has been shown that the TIE correctly reconstructs the modified phase of electromagnetic waves in the light-optical regime [7]. The TIE has been shown to successfully retrieve the phase for coherent and partially coherent illumination [8].

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Approximating the measurement of the variation of the irradiance along the optical axis by a finite difference approach is a severe limitation to the accuracy of phase measurements by the TIE, making it valid for a only a limited range of spatial frequencies [9]. Although higher order intensity derivatives can be used to provide more accurate estimates for the variation of irradiance along the optical axis [10,9], another problem of the TIE, the fact that the boundary conditions are not defined (see below) still remains. Non-linear wave function retrieval [11–14], on the other hand, uses the full mathematical expression describing the propagation of wave functions in free space and can thus be self-consistent and more reliable at much larger Fresnel numbers. However, in comparison to such non-linear methods the TIE allows 'extrapolation' of phase information to much lower spatial frequencies (i.e. it infers long-range phase information from very local measurements), making it a suitable method for medium resolution imaging [15]. Different hybrid approaches to combine the advantages of the TIE with those of non-linear reconstruction schemes extend the validity of the TIE to larger bands of spatial frequencies [16,17].

The most popular technique for solving the TIE is based on the Fast Fourier Transform (FFT), since the Laplacian reduces to a simple product with $\left|\vec{q}\right|^2$ in reciprocal space [8], where $\vec{q} = \left(q_x, q_y\right)$ is the coordinate in reciprocal space. An alternative method for solving the TIE directly in real space is multi-grid numerical integration [18]. The problem common to all these approaches is that the necessary boundary conditions (BCs) are not known. FFT based methods solve the TIE non-iteratively in the frequency domain by implicitly assuming periodic BCs in the phase. This assumption is only valid in rare cases. Mirror padding extends the FFT approach, providing a way for imposing a special case of Neumann and Dirichlet boundary conditions [19]. Multi-grid based approaches have been shown to yield an exact solution of the TIE in the spatial domain iteratively in the presence of the periodic boundary conditions [20].

In this paper, we first review how the TIE is directly linked to the Helmholtz equation and introduce a new combination of flux-preserving and Dirichlet boundary condition based on prior knowledge of regions of constant phase in the image plane (e.g. a region not covered by the object, or a hole in the object). The advantage of the proposed combination of boundary conditions lies in the ability to reconstruct wave fronts also in case we cannot make any reasonable assumption of the boundary conditions on the outer edge of the field of view (e.g. where the assumption of periodic BCs is not justified). We apply a finite-element multi-grid based calculation applying above-mentioned boundary condition and also the FFT approach to experimental optical data and compare the results.

2. Theory

We define a scalar monochromatic wave travelling primarily along the z-direction as [21]

$$\psi\left(\vec{r}_\perp, z\right) = A\left(\vec{r}_\perp, z\right)\exp\left(ikz\right) \tag{1}$$

where $k = 2\pi/\lambda$ is the wavenumber, and $\vec{r}_\perp$ is a vector in the plane perpendicular to the z-direction. The Helmholtz equation in three dimensional Cartesian coordinates for the propagation of a wave in free space is given by [21]

$$\left(\nabla^2 + k^2\right)\psi\left(\vec{r}_\perp, z\right) = 0 \tag{2}$$

where ∇^2 is the three-dimensional Laplace operator. Assuming that the complex envelope $A\left(\vec{r}_\perp, z\right)$ of the wave changes slowly in the direction of propagation, z, i.e. $\partial^2 A/\partial z^2 << k^2 A$, one can derive the following parabolic equation by substituting (1) into (2)

$$\left(\frac{\nabla_\perp^2}{2k} + i\frac{\partial}{\partial z} + k\right)\left[A\left(\vec{r}_\perp, z\right)\exp\left(ikz\right)\right] = 0 \tag{3}$$

The complex envelope of the wave in (1) may be defined in terms of the intensity I and a phase φ as

$$A\left(\vec{r}_\perp, z\right) = \sqrt{I\left(\vec{r}_\perp, z\right)}\exp\left(i\varphi\left(\vec{r}_\perp, z\right)\right) \tag{4}$$

Substituting $A\left(\vec{r}_\perp, z\right)$ in (3) for the right hand side of (4), and considering only the imaginary parts on either side yields the so-called the TIE

$$\vec{\nabla}_\perp\cdot\left[I\left(\vec{r}_\perp, z\right)\vec{\nabla}_\perp\varphi\left(\vec{r}_\perp, z\right)\right] = -k\frac{\partial I\left(\vec{r}_\perp, z\right)}{\partial z} \tag{5}$$

The TIE is a second-order, elliptical partial differential equation which, for properly defined boundary conditions of the phase $\varphi\left(\vec{r}_\perp, z\right)$ and noise-free data has a unique solution (up to an additive constant in case of periodic or Neuman BCs) for strictly positive intensity [22]. Points with zero intensity may be associated with discontinuities in the phase map [23], in which case unique phase information cannot be retrieved (but see [24] in the case of vortices with known orbital angular momentum).

Comparing the TIE with the differential form of the continuity equation suggests that $I\left(\vec{r}_\perp, z\right)\vec{\nabla}_\perp\varphi\left(\vec{r}_\perp, z\right)$ expresses the flux of intensity along the direction of propagation or the transverse component of the Poynting vector. Hence, the transverse component of the Poynting vector can be written as

$$\vec{S}_\perp = I\left(\vec{r}_\perp, z\right)\vec{\nabla}_\perp\varphi\left(\vec{r}_\perp, z\right) \tag{6}$$

Integrating both sides of (5) over the field of view $D(x, y)$ bounded by the perimeter P and applying the two-dimensional Green's theorem to the left hand side leads us to an expression for the amount of flux lost or gained at the boundaries

$$\int\int_D\left(\vec{\nabla}_\perp\cdot\vec{S}\right)dA = \oint_P \vec{S}\cdot\hat{n}\, dP \tag{7}$$

Here $\hat{n}$ symbolises the unit vector normal to the boundaries in the detection plane. Described already in the work of Tegue [5], conservation of intensity is assumed for the TIE to have a unique solution

$$\int\int_D \partial_z I\left(x, y\right) dA = \oint_P \vec{S}.\,\hat{n}\, dP \tag{8}$$

which states that the conservation of intensity is valid if the amount of flux crossing the boundaries is zero. Combining (8) with (6) yields the Neumann boundary condition [19]

$$\frac{\partial\varphi(P)}{\partial\hat{n}} = 0 \tag{9}$$

As stated above, computation of the intensity variation along the optical axis $\partial_z I(x, y)$ requires measuring images at different planes of focus. Typically image intensities are detected at the following three planes of focus: $f = -\Delta f,\ 0, +\Delta f$, where $f=0$ is the in-focus image and Δf is some fixed defocus step. In practice, when acquiring images under different defocus values intensity is not preserved. Therefore, a straightforward solution to the TIE does not generally exist. In order to overcome mentioned obstacle, we pad the experimental images with the overall mean value of the experimental data by embedding the images into much larger