Numerical Techniques for Optical Diffraction

Abstract— **Diffraction is a characteristic of wave phenomena that occurs when a propagating wavefront is obstructed by a medium. It is applied in phase imaging and to model wave propagation in optical instruments and imaging systems by solving the diffraction integral. Diffraction theory has been discussed extensively by existing literature. However, most of these only focus on certain aspects of diffraction theory and the challenges associated with numerical implementation such as pixel size variation, amplitude scaling, diffraction associated with transparent structures are glossed over superficially. In addition, most of the work reported lie scattered throughout the literature. This article serves two purposes, a) to provide the essential details of diffraction theory at one place, thereby making it easily accessible for readers; b) to provide open source algorithms (named OpenDiffraction) for the various numerical techniques discussed in this paper, which enables users to interactively vary the code parameters and study it's effect on the diffraction pattern.**

Index Terms **- Diffraction, 2D Fourier Transform**

I. INTRODUCTION

When a propagating wavefront encounters an obstacle, it bends around the edges of the obstacle and this phenomenon is known as Diffraction. In the course of encountering a diffracting structure, either transparent or opaque, the amplitude and/or phase of a portion of the wavefront is altered. The diffracting structure effectively becomes a secondary source of propagating wavelets in accordance with the Huygens-Fresnel principle . The wavelets that continue to propagate beyond the obstacle will interfere with each other resulting in a particular energy-density distribution known as the diffraction pattern.

After a considerable distance of propagation, the spherical waves can be approximated as planar waves and Fraunhofer diffraction obtains. On the other hand, if the observation plane is closer to the source plane containing the diffracting structure, the planar approximation cannot be made and a Fresnel diffraction pattern would exist.

II. WAVE-MATTER INTERACTION

To model wave propagation, it is essential to understand how a propagating wave is modified upon interacting with matter. A coherent monochromatic plane wave with a wavelength λ and an intensity profile $I_o(x,y)$ propagating in the +z-direction can be represented as

$$U_o(x,y;z) = \sqrt{I_o(x,y)}\ e^{-jkz}$$

where $k = \frac{2\pi}{\lambda}$ is the angular wave-number. The relation between the complex amplitude, U, and intensity, I, of an optical wave is , $I(x,y) = |U(x,y)|^2$.

A. Interaction with transparent objects

When the wave passes through an object, its amplitude and/or phase gets altered. Such objects are called phase objects and can be described by its complex refractive index,

$$n = 1 - \alpha - i\beta$$

Within the object, the angular wave-number changes from k to nk and the wave can be described as,

$$\begin{aligned} U_1(x,y,z) &= \sqrt{I_o(x,y)}\ e^{-jnkz} \\ &= \sqrt{I_o(x,y)}\ e^{-ikz}\ e^{i\alpha kz}\ e^{-\beta kz} \\ &= \sqrt{I_o(x,y)}\ e^{-ikz}\ e^{i\phi(x,y)} \sqrt{T(x,y)} \end{aligned}$$

If the object has a thickness L(x,y), then $\phi(x,y) = \alpha k\ L(x,y)$ is the phase shift and $T = e^{-2\beta kL(x,y)}$ is the exponential decay in the intensity of the light. Thus, the complex amplitude in the source plane at z = 0 is,

$$U_1(x,y) = \sqrt{I_o(x,y)T(x,y)}\ \ e^{j\phi(x,y)}$$

The phase and transmission profile for two overlapped partially absorbing spheres with radii R_1 and R_2 and center points at C_1 and C_2 respectively with the below parameters are shown in Fig. 1 and Fig. 2.

Parameter	Value
λ	500 nm
α_1,α_2	0.001
β_1,β_2	0.00002
R_1	2.3 mm
R_2	1.4 mm
C_1	(0,0)
C_2	(-1.5 mm,0)

Parameters for a two-ball object

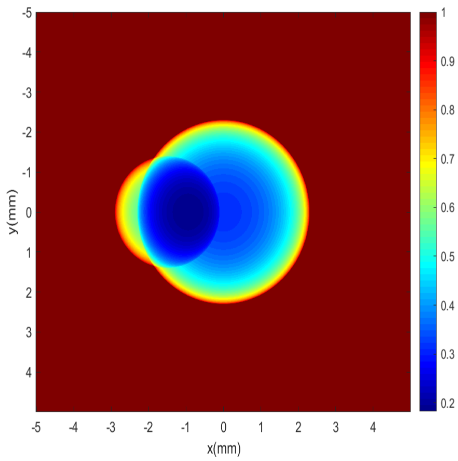

Fig. 1: Transmission, T(x,y)=$T_1(x,y) \times T_2(x,y)$

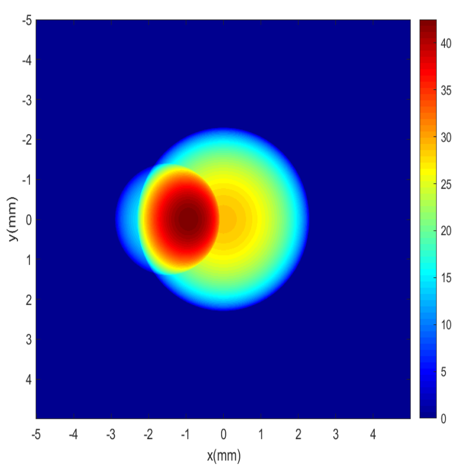

Fig. 2: Phase, $\phi(x,y) = \phi_1(x,y) + \phi_2(x,y)$

B. Interaction with opaque objects

When the wave interacts with an opaque screen with aperture(s), only its intensity is modified and phase is unchanged. The opaque object can be described by a transmission function which is constant for light of all wavelengths. In case of an opaque screen with a circular aperture of radius R= 1mm centred at the origin, the transmission function can be described as,

$$T(x,y) = \begin{cases} 1, & \text{if } \sqrt{x^2+y^2} \leq R \\ 0, & \text{otherwise} \end{cases}$$

The complex amplitude at the z=0 plane is

$$U_1(x,y) = \sqrt{I_o(x,y)T(x,y)}$$

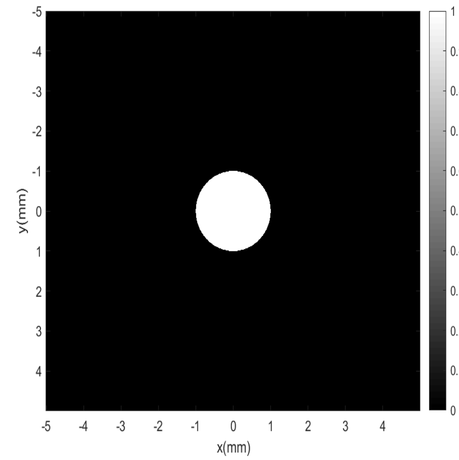

Fig. 3: Transmission, T(x,y)

III. Diffraction Theory

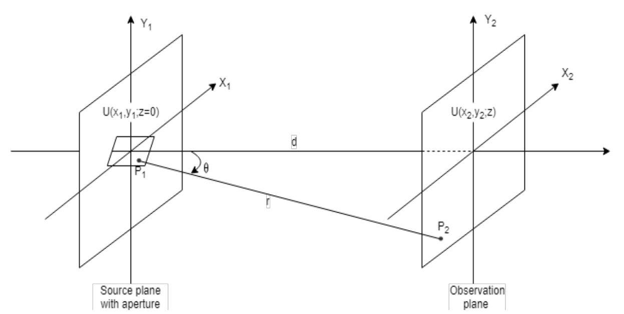

Fig. 4: Diffraction geometry.

The z=0 plane is the source plane and the source plane field is propagated to a parallel plane at z=d, which is termed the observation plane. The source plane co-ordinates are represented by $r_1 = (x_1, y_1)$ and the observation plane co-ordinates are represented by $r_2 = (x_2, y_2)$. θ is the angle between a vector perpendicular to the source plane and the vector 'r' joining the points P1 and P2. With the known source plane field, the observation plane field is obtained using Huygens's principle,

$$U(x_2,y_2) = \frac{1}{i\lambda} \iint_\Sigma U(x_1,y_1) \frac{e^{ikr}}{r} \cos\theta \quad dx_1\,dy_1 \tag{1}$$

'Σ' represents the diffracting structure.

By observing the diffraction geometry, $\cos\theta = \frac{d}{r}$.

$$U(x_2,y_2) = \frac{d}{i\lambda}\iint_{\Sigma} U(x_1,y_1)\frac{e^{ikr}}{r^2}\quad dx_1\,dy_1 \tag{2}$$

The distance between the points P_1 and P_2 is,

$$r = \sqrt{d^2+(x_2^2-x_1^2)+(y_2^2-y_1^2)}$$

By factoring 'd' outside the square root in the above equation and expanding 'r' as a Taylor series and retaining only the first two terms of the expansion, the Fresnel approximation is obtained as,

$$r \approx d\left[1+\frac{1}{2}\left(\frac{x_2-x_1}{d}\right)^2+\frac{1}{2}\left(\frac{y_2-y_1}{d}\right)^2\right]$$

'r' in the denominator of (2) can be approximated as z. In the exponent, however, the approximation cannot be made, as phase changes of even a fraction can alter the value of this exponential term by a large amount.

Thus, the expression known as the Fresnel diffraction integral is obtained

$$U(x_2,y_2) = \frac{e^{ikd}}{i\lambda d}\iint_{\Sigma} U(x_1,y_1)e^{\frac{ik}{2d}[(x_2-x_1)^2+(y_2-y_1)^2]}\,dx_1\,dy_1 \tag{3}$$

IV. Fresnel diffraction Integral and its forms

A. *Fourier Transform computation*

The squared terms in the exponential of the Fresnel diffraction integral can be expanded and the term $exp(\frac{ik}{2d}(x_2^2+y_2^2))$ is factored to yield

$$U(x_2,y_2) = A\iint_{-\infty}^{+\infty}\{U(x_1,y_1)\times B\}e^{-i2\pi\left(\frac{x_2}{\lambda d}x_1+\frac{y_2}{\lambda d}y_1\right)}\quad dx_1\,dy_1$$

Where,

$$A = \frac{e^{ikd}}{i\lambda d}e^{\frac{ik}{2d}(x_2^2+y_2^2)} \qquad\qquad B = e^{\frac{ik}{2d}(x_1^2+y_1^2)}$$

which can be evaluated as a single 2D Fourier transform

$$U(x_2,y_2) = \frac{e^{ikd}e^{\frac{ik}{2d}(x_2^2+y_2^2)}}{i\lambda d}\mathscr{F}\left\{U(x_1,y_1)e^{\frac{ik}{2d}(x_1^2+y_1^2)}\right\}\Bigg|_{f_{x_1},f_{y_1}} \tag{4}$$

evaluated at spatial frequencies,

$$f_{x_1} = \frac{x_2}{\lambda d} \tag{5}$$ $$f_{y_1} = \frac{y_2}{\lambda d} \tag{6}$$

The complex amplitude $U(x_2,y_2)$ must be scaled to satisfy conservation of energy. This scaling factor is required because of the transform from the spatial to frequency domain. The scaling factor is computed using Parseval's theorem which states that if $\mathscr{F}\{g(x,y)\} = G(f_x,f_y)$, then:

$$\sum\sum_{-\infty}^{\infty}|g(x,y)|^2dxdy = \sum\sum_{-\infty}^{\infty}|G(f_x,f_y)|^2df_xdf_y$$

the integral of the square of a function is equal to the integral of the square of its transform. Here, $g(x,y) = U(x_1,y_1)e^{\frac{ik}{2d}(x_1^2+y_1^2)}$. The amplitude scaling factor is,

$$C(x_1,y_1) = \sqrt{\frac{\sum\sum_{\Sigma}\left|U(x_1,y_1)e^{\frac{ik}{2d}(x_1^2+y_1^2)}\right|^2dx_1dy_1}{\sum\sum_{\Sigma}\left|\mathscr{F}\left\{U(x_1,y_1)e^{\frac{ik}{2d}(x_1^2+y_1^2)}\right\}\right|^2df_{x_1}df_{y_1}}} \tag{7}$$

The scaled wave-field in the observation plane is obtained by,

$$U(x_2,y_2) = FRT\{U(x_1,y_1)\}\times C(x_1,y_1) \tag{8}$$

FRT represents the Fresnel transform operation in Eq.(4)

B. *Convolutional computation*

Alternatively, Eq.(3) can be expressed in the form of a convolution as:

$$U(x_2,y_2) = \iint_{-\infty}^{+\infty}U(x_1,y_1)h(x_2-x_1,y_2-y_1)\quad dx_1\,dy_1$$

Where the free-space convolution kernel is given by,

$$h(x_1,y_1) = \frac{e^{ikd}e^{\frac{ik}{2d}(x_1^2+y_1^2)}}{i\lambda d}$$

$$\Longrightarrow U(x_2,y_2) = U(x_1,y_1)\circledast\frac{e^{ikd}e^{\frac{ik}{2d}(x_1^2+y_1^2)}}{i\lambda d} \tag{9}$$

Convolution theorem is applied to yield,

$$U(x_2,y_2) = \mathscr{F}^{-1}\left\{\mathscr{F}\{U(x_1,y_1)\}\times H\right\} \tag{10}$$

Where,

$$H = \mathscr{F}\left\{\frac{e^{ikd}e^{\frac{ik}{2d}(x_1^2+y_1^2)}}{i\lambda d}\right\} = e^{-i\pi\lambda d(f_{x_1}^2+f_{y_1}^2)} \tag{11}$$

Since an inverse Fourier transform is performed to compute the observation plane field, scaling is not required here.

V. Numerical implementation of Fresnel diffraction integral

In this section, numerical methods for evaluating the two forms of Fresnel diffraction integral using equations (8) and (10) are discussed. To evaluate the equations on a computer, a sampled version of the source plane field U(x_1,y_1) must be used. The source plane grid has N sample points in each direction and the grid spacing is δ_1. Similarly, the observation plane has N sample points and has a grid spacing of δ_2.

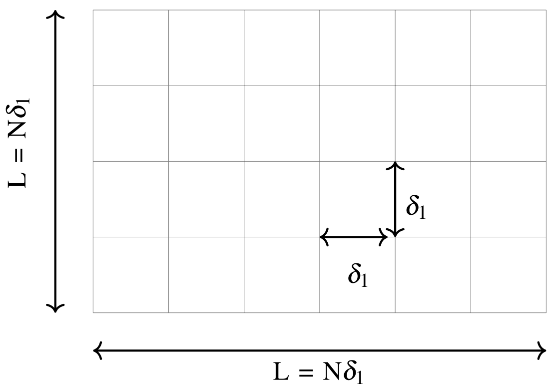

Fig. 5: Source plane grid

Parameter	Value
N	2048
L	10 mm
δ_1	2.44140625 μm

A. Fourier Transform representation

This section describes two methods of implementing the Fourier transform representation of the Fresnel diffraction integral in the form of Eq. (8). The first method evaluates this integral once as a single FT, which is the most straightforward. This method is desirable because of its computational efficiency. The second method evaluates the Fresnel integral twice, which adds some flexibility in the grid spacing at the cost of performing a second FT.

V-A.1 One -step propagation

The complex field in the source plane at z = 0 for the phase object with two partially absorbing spheres is directly propagated to the observation plane at z=d.

By using (5) and (6), it is straightforward to deduce that

$$\delta_{f_1} = \frac{\delta_2}{\lambda d}$$

The spacing in the frequency domain of the source plane is $\delta_{f_1} = \frac{1}{N\delta_1}$.

$$\implies \delta_2 = \frac{\lambda d}{N\delta_1} \tag{12}$$

The above expression is utilized to compute the observation plane grid co-ordinates (x_2, y_2) and Eq.(8) is implemented to determine the observation plane field $U(x_2, y_2)$.

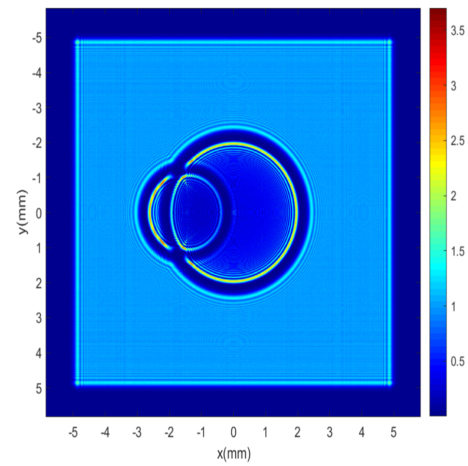

Fig. 6: Intensity pattern at z= 0.05m (with scaling)

From (12), it is obvious that the we have no control over spacing in the observation plane grid spacing. For a given N, λ, δ_1 , the value of δ_2 changes with variation in d. This is illustrated in the following figure by varying the propagation distance

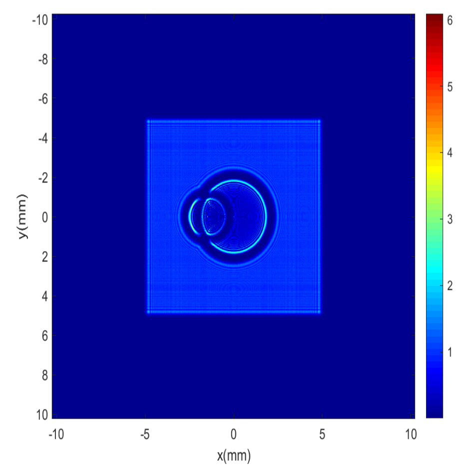

Fig. 7: Intensity pattern at z= 0.1m

The varying observation plane dimension is addressed in the following section. In-addition, to avoid aliasing in the observation plane and to satisfy the Nyquist criterion, for a given N and δ_1, the propagation distance should be such that,

$$d \geq 2\frac{D_1\delta_1}{\lambda} \tag{13}$$

D_1 is the maximum spatial extent of the illuminating field. For the example of phase object, $D_1 = N\delta_1$ and for the source plane with a circular aperture of radius R, $D_1 = 2R$.

V-A.2 Two step propagation

To provide flexibility to choose the observation plane grid spacing, a scaling parameter, '$s = \frac{\delta_2}{\delta_1}$', is introduced. In two-step propagation method, the source plane field $U(x_1, y_1)$ is propagated to an intermediate plane at $z = d_i$ and then the intermediate plane field is propagated to the observation plane at $z = d$. The value for d_1 can be chosen such that 'm' has the desired value. The geometry for the two-step propagation is shown in Fig.9. The grid spacing in the intermediate plane is

$$\delta_i = \frac{\lambda d_1}{N\delta_1}$$

$$\implies \delta_2 = \frac{\lambda d_2}{N\delta_i} = \frac{\lambda d_2}{N(\frac{\lambda d_1}{N\delta_1})} = \frac{d_2}{d_1}\delta_1 = s\delta_1$$

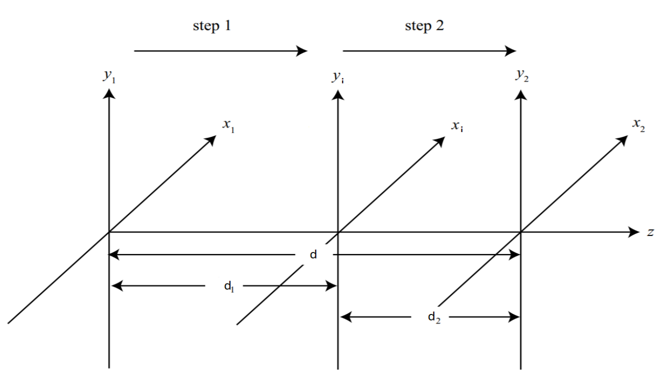

Fig. 8: Diffraction geometry

The propagation distances are,

$$d_1 = \frac{d}{s+1}$$
$$d_2 = d - d_1$$

Thus, a choice of 's' defines the location of the intermediate plane.

$$U(x_i, y_i) = FRT\{U(x_1, y_1)\} \times C(x_1, y_1);$$
$$U(x_2, y_2) = FRT\{U(x_i, y_i)\} \times C(x_i, y_i);$$

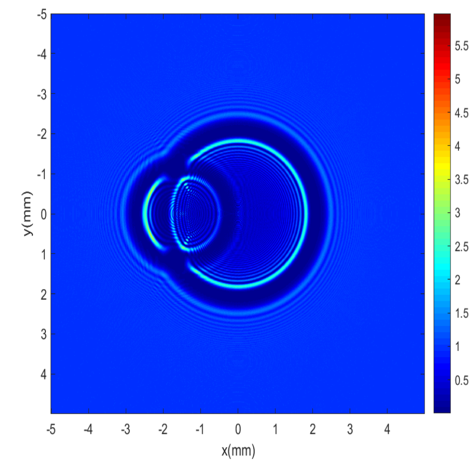

Fig. 9: Intensity pattern at z=0.1m; s=1

B. Convolution representation

In this section, the convolution form of the Fresnel diffraction integral in Eq. (10) is numerically evaluated. In this method, the grid spacings are such that $\delta_1 = \delta_2$ by default. To provide flexibility with choosing the observation plane grid spacing, [3] and [4] proposed a method to introduce the scaling parameter s=δ_2/δ_1 into the Fresnel diffraction integral by rewriting Eq.(3) using $r_2 = (x_2, y_2)$ and $r_1 = (x_1, y_1)$

$$U(r_2) = \frac{e^{ikd}}{i\lambda d}\int_{-\infty}^{+\infty} U(r_1)\, e^{\frac{ik}{2d}|\vec{r}_2-\vec{r}_1|^2}\, dr_1 \tag{14}$$

By applying the rule for a norm associated to a scalar product,

$$|\vec{r}_2 - \vec{r}_1|^2$$

$$= |\vec{r}_2|^2 - 2\vec{r}_2.\vec{r}_1 + |\vec{r}_1|^2$$

$$= \left(|\vec{r}_2|^2 + \frac{|\vec{r}_2|^2}{s} - \frac{|\vec{r}_2|^2}{s}\right) - 2\vec{r}_2.\vec{r}_1 + (|\vec{r}_1|^2 + m|\vec{r}_1|^2 - s|\vec{r}_1|^2)$$

$$= s\left|\frac{\vec{r}_2}{s} - \vec{r}_1\right|^2 - \frac{1-s}{s}|\vec{r}_2|^2 + (1-s)|\vec{r}_1|^2$$

and applying it to Eq.(14)

$$U(r_2) = \frac{e^{ikd}}{i\lambda d} e^{\frac{-jk(1-s)}{2d}\frac{|\vec{r_2}|^2}{s}} \int_{-\infty}^{+\infty} U(r_1) e^{\frac{jk(1-s)}{2d}|\vec{r_1}|^2} e^{\frac{jks}{2d}|\frac{\vec{r_2}}{s}-\vec{r_1}|^2} dr_1$$

The convolution integral can be obtained by defining

$$A(r_1) = \frac{U(r_1)}{s} e^{\frac{jk(1-s)}{2d}|\vec{r_1}|^2}$$

$$\Longrightarrow U(r_2) = \frac{e^{ikd}}{i\lambda(\frac{d}{s})} e^{\frac{-jk(1-s)}{2(\frac{d}{s})}\left(\frac{|\vec{r_2}|}{s}\right)^2} \int_{-\infty}^{+\infty} A(r_1) e^{\frac{jks}{2d}|\frac{\vec{r_2}}{s}-\vec{r_1}|^2} dr_1$$

$$= e^{\frac{-jk(1-s)}{2(\frac{d}{s})}\left(\frac{|\vec{r_2}|}{s}\right)^2} \int_{-\infty}^{+\infty} A(r_1) h(\frac{r_2}{s} - r_1) dr_1$$

$$= e^{\frac{-jk(1-s)}{2(\frac{d}{s})}\left(\frac{|\vec{r_2}|}{s}\right)^2} [A(r_1) \circledast h(r_1)]$$

with the convolution kernel given by,

$$h(r_1) = \frac{e^{ikd}}{i\lambda(\frac{d}{s})} e^{\frac{jks}{2d}|\vec{r_1}|^2}$$

By applying convolution theorem,

$$U(x_2, y_2) = e^{\frac{-jk(1-s)(x_2^2+y_2^2)}{2sd}} \mathscr{F}^{-1}\left\{ \mathscr{F}\{A(r_1)\} e^{\frac{-i\pi\lambda(f_{x_1}^2+f_{y_1}^2)d}{s}} \right\}$$

To avoid aliasing in the observation plane, the propagation distance should be such that,

$$d \leq \frac{N\delta_1\delta_2}{\lambda} \tag{15}$$

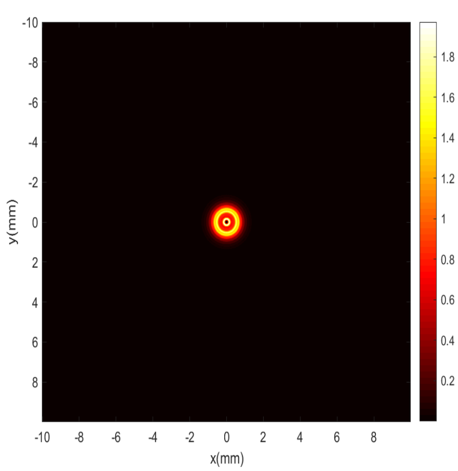

Fig. 10: Intensity pattern at z= 0.5m; s= 2

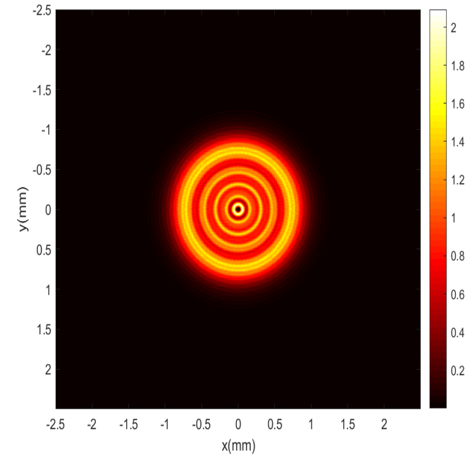

Fig. 11: Intensity pattern at z= 0.2m; s= 0.5

VI. Conclusion

In this paper, a compilation of numerical techniques for diffraction were provided. The techniques were illustrated for both transparent and opaque objects. In addition, the issues of amplitude scaling and observation grid spacing were addressed. It was shown that Angular spectrum method can be used for near-field applications and Fresnel transform method can be applied for propagating to larger distances

References

[1] Jason D. Schmidt, "Numerical Simulation of Optical Wave Propagation",SPIE ,Bellingham, Washington . 2010. Digital

[2] G. A. Tyler and D. L. Fried, "A wave optics propagation algorithm," Tech. Rep. TR-451, the Optical Sciences Company (1982).

[3] P. H. Roberts, "A wave optics propagation code," Tech. Rep. TR-760, the Optical Sciences Company (1986).

[4] N. Streibl, "Phase imaging by the transport equation of intensity," Opt. Commun. 49(1), 6–10 (1984).

[5] M. Born and E. Wolf, Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light, 7th Ed., Cambridge University Press (1999).

[6] Y.Zhu, Z.Zhang, and G.Barbastathis, "Phase imaging for absorptive phase objects using hybrid uniform and structured illumination Transport of Intensity Equation", Optics Express, pp. 28966-28976 (2014) .

[7] Wikipedia contributors. "Phase-contrast X-ray imaging." Wikipedia, The Free Encyclopedia. Wikipedia, The Free Encyclopedia, 6 Oct. 2019.

[8] T.C.Poon, JP Liu. "Introduction to Modern Digital Holography". Cambridge University Press, New York , 2014 Year Published. Print.

[9] Bahaa E.A, Saleh, M.C Teich, "Fundamentals of Photonics". John Wiley sons, Inc. New york, 1991. Print

[10] J. W. Goodman, Introduction to Fourier Optics, 3rd Ed., Roberts Co., Greenwood Village, CO (2005)

[11] N. Delen and B. Hooker, "Free-space beam propagation between arbitrarily oriented planes based on full diffraction theory: a fast Fourier transform approach," J. Opt. Soc. Am. A 15(4), pp. 857–867 (1998).