Numerical Techniques for Diffraction

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Abstract— **Diffraction is a characteristic of wave phenomena that occurs when a propagating wavefront is obstructed by a medium. It has many applications such as phase imaging, wave propagation modelling in optical instruments and imaging systems. While the existing literature covers the basic implementation of the numerical techniques for diffraction, the key elements such as pixel size variation, amplitude scaling, diffraction associated with transparent structures are under-emphasized. This article serves two purposes: a) to provide the essential details of diffraction theory in one place, thereby making it easily accessible for readers; b) to provide open source algorithms (named OpenDiffraction)to provide an in-depth understanding of the various numerical techniques discussed in this paper.**

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

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 spherical wavelets in accordance with the Huygens-Fresnel principle . The wavelets that propagate beyond the obstacle will interfere with each other resulting in a particular energy-density distribution known as the diffraction pattern [7].

Diffraction can be classified into two types namely Fresnel and Fraunhofer diffraction depending on the propagation distance. Fresnel diffraction occurs in the near field whereas Fraunhofer diffraction occurs at the far-field. In this article, only the numerical techniques for Fresnel diffraction are discussed. Since Fraunhofer diffraction is essentially an approximation of the Fresnel diffraction, the techniques for the former can be applied to the latter.

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 [7]

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

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 [9], $I(x,y) = |U(x,y)|^2$.

A. Interaction with phase objects

When the wave passes through a phase object, its phase and/or phase gets altered. Such objects are described by their complex refractive index [5],

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

Where the decrement of the real part of the refractive index α contributes to the phase shift of the incident wave and the absorption coefficient β attenuates the wave. Within the object, the angular wave-number changes from k to nk and the modified wave is,

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

If the object has a thickness $L_t(x,y)$, then $\phi(x,y) = \alpha k\, L_t(x,y)$ is the phase shift and $T = e^{-2\beta k L_t(x,y)}$ is the exponential decay in the intensity of the light. 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 half ball lenses 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

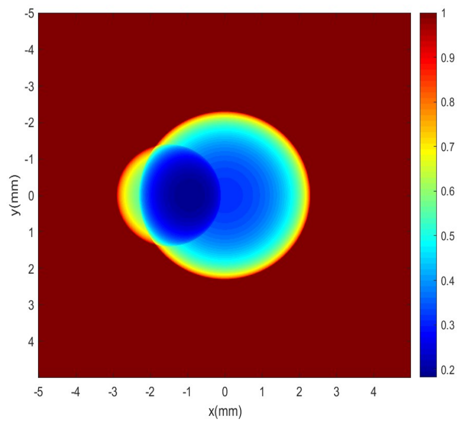

Fig. 1: Transmission, T(x,y)=$T_1(x,y) \times T_2(x,y)$

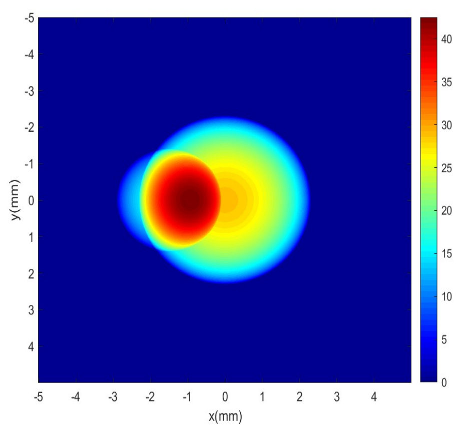

Fig. 2: Phase, $\phi(x,y) = \phi_1(x,y) + \phi_2(x,y)$

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

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

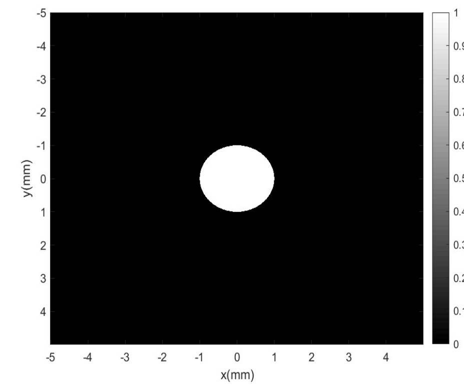

Fig. 3: Transmission, T(x,y)

III. Diffraction Theory

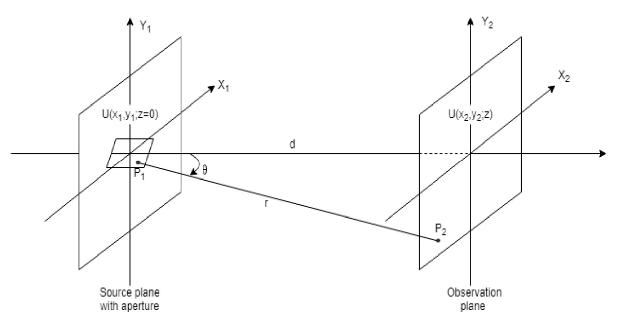

Fig. 4: Diffraction geometry.

The source plane field at z=0 is propagated to a parallel observation plane at z=d. 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,[7]

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

'Σ' represents the diffracting structure.

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

$$U(x_2,y_2) = \frac{d}{i\lambda}\iint_{\Sigma} U(x_1,y_1)\frac{e^{ikr}}{r^2} \quad dx_1\,dy_1 \tag{1}$$

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' using Taylor series expansion, the Fresnel approximation is obtained by discarding every term except the first two to give,

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

'r' in the denominator of (1) can be approximated as z. However, this approximation cannot be applied inside the exponent in (1) as even a fractional value of change in the phase could alter the value of the exponent significantly.

The Fresnel diffraction integral is obtained as,

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

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[9]

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

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

$$U(x_2,y_2) = \frac{e^{ikd}e^{\frac{ik}{2d}(x_2^2+y_2^2)}}{i\lambda d}\mathscr{F}\left\{U(x_1,y_1)e^{\frac{ik}{2d}(x_1^2+y_1^2)}\right\}\Bigg|_{f_{x_1},f_{y_1}} \tag{3}$$

evaluated at spatial frequencies,

$$f_{x_1} = \frac{x_2}{\lambda d} \quad (4) \qquad\qquad f_{y_1} = \frac{y_2}{\lambda d} \quad (5)$$

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[3] 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,

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

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

$$U(x_2,y_2) = FRT\{U(x_1,y_1)\}\times C(x_1,y_1) \tag{6}$$

FRT represents the Fresnel transform operation in Eq.(3)

B. *Convolutional computation*

Alternatively, Eq.(3) can be expressed as a convolution:[1]

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

Where the free-space convolution kernel is given by,

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

$$\implies U(x_2,y_2) = U(x_1,y_1)\circledast h(x_1,y_1)$$

Convolution theorem is applied to yield,

$$U(x_2,y_2) = \mathscr{F}^{-1}\left\{\mathscr{F}\{U(x_1,y_1)\}\times H\right\} \tag{7}$$

Where,

$$H = \mathscr{F}\left\{\frac{e^{ikd}e^{\frac{ik}{2d}(x_1^2+y_1^2)}}{i\lambda d}\right\} = e^{-i\pi\lambda d(f_{x_1}^2+f_{y_1}^2)} \tag{8}$$

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 (6) and

(8) are discussed. The source plane field U(x_1,y_1) is sampled to be evaluated in a computer. The source plane grid has N sample points in each direction and a pixel size δ_1. Similarly, the observation plane has N sample points and a pixel size δ_2. For simplicity, it is assumed that the grid is composed of square pixels.

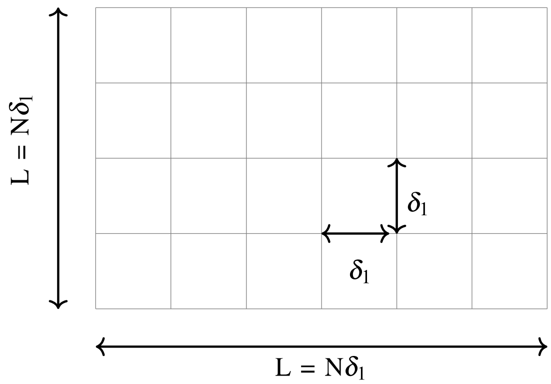

Fig. 5: Source plane grid

Parameter	Value
N	2048
L	10 mm
δ_1	2.44 μm

A. Fourier Transform computation

In this section, a numerical method for simulating diffraction using the Fourier transform representation of the Fresnel diffraction integral in Eq. (6) is discussed. The first method involves only a single Fourier transform computation but does not provide flexibility in choosing the observation plane pixel size.

V-A.1 One plane propagation

The source plane field located at z = 0 for the phase object with two partially absorbing spheres is directly propagated to the observation plane at z =d.[1]

By using (4) and (5), 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 δ_{f_1}=$\frac{1}{N\delta_1}$.

$$\implies \delta_2 = \frac{\lambda d}{N\delta_1} \tag{9}$$

The above expression is utilized to compute the observation plane grid co-ordinates (x_2, y_2) and Eq.(6) is implemented to determine the observation plane field $U(x_2, y_2)$.

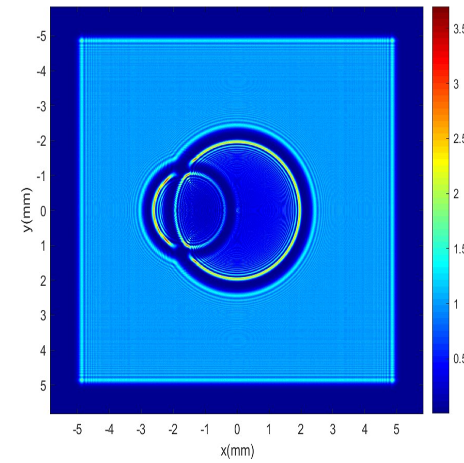

Fig. 6: Intensity pattern at d= 0.05m (with amplitude scaling)

From (9), it is observed that for a given N, λ, δ_1 , the value of δ_2 increases with variation in d. This is illustrated in the following figure by varying the propagation distance

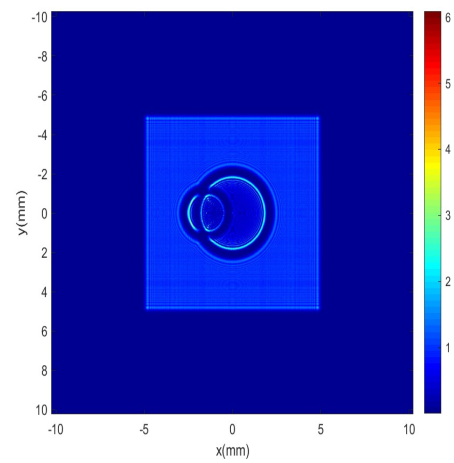

Fig. 7: Intensity pattern at d= 0.1m

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, [1]

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

D_1 is the extent of the object in the spatial domain. For the two ball phase object, $D_1 = N\delta_1$ and for the circular aperture of radius R, $D_1 = 2R$.

V-A.2 *Two Plane propagation*

To provide flexibility in choosing the observation plane pixel size, a two plane propagation method can be used[4][8]. In this method, the source plane field $U(x_1,y_1)$ is propagated to a plane interposed between the planes z=0 and z=d. This intermediate field is then propagated to the observation plane at $z=d$. The parameter $s=\frac{\delta_2}{\delta_1}$ is the ratio of the pixel size in the observation plane and the source plane. The geometry for the two-plane propagation is shown in Fig. 9. The pixel size in the interposed plane is

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

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

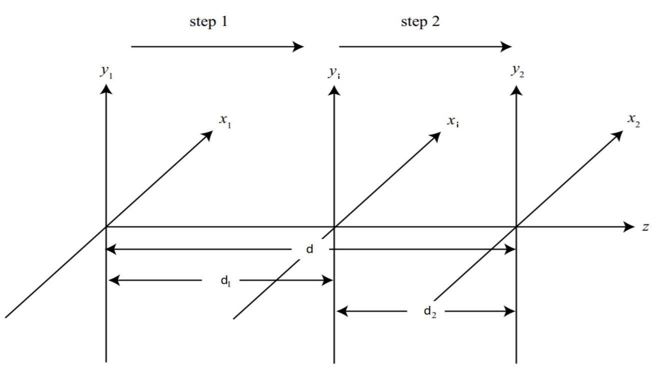

Fig. 8: Diffraction geometry

The propagation distances are,

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

$$d_2 = d - d_1$$

$$d = d_1 + d_2$$

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

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

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

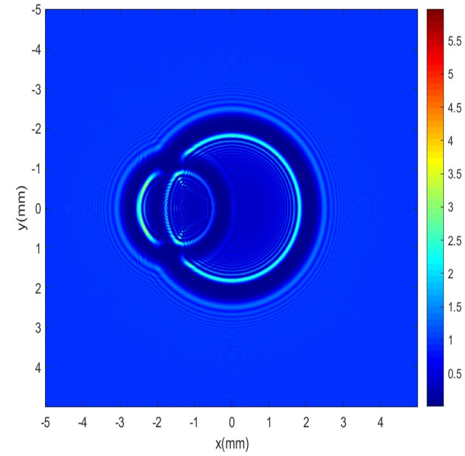

Fig. 9: Intensity pattern at d = 0.1m; s=1

B. *Convolution computation*

The convolution representation of the Fresnel diffraction integral in Eq. (8) is numerically evaluated in this section. In this method, the pixel sizes are such that $\delta_1 = \delta_2$ by default. To provide flexibility with choosing the observation plane pixel size, [2] and [6] proposed a method to introduce the scaling parameter s=δ_2/δ_1 into the Fresnel diffraction integral by rewriting Eq.(2) using $r_2 = (x_2,y_2)$ and $r_1 = (x_1,y_1)$

$$U(r_2) = \frac{e^{ikd}}{i\lambda d}\int_{-\infty}^{+\infty} U(r_1)\, e^{\frac{ik}{2d}|\vec{r_2}-\vec{r_1}|^2}\, dr_1 \tag{10}$$

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

$$\begin{aligned}
&|\vec{r_2}-\vec{r_1}|^2 \\
&= |\vec{r_2}|^2 - 2\vec{r_2}.\vec{r_1} + |\vec{r_1}|^2 \\
&= \left(|\vec{r_2}|^2 + \frac{|\vec{r_2}|^2}{s} - \frac{|\vec{r_2}|^2}{s}\right) - 2\vec{r_2}.\vec{r_1} + (|\vec{r_1}|^2 + m|\vec{r_1}|^2 - s|\vec{r_1}|^2) \\
&= s\left|\frac{\vec{r_2}}{s} - \vec{r_1}\right|^2 - \frac{1-s}{s}|\vec{r_2}|^2 + (1-s)|\vec{r_1}|^2
\end{aligned}$$

and applying it to Eq.(10)

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

The convolution integral can be obtained by defining

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

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

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

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

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,[1]

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

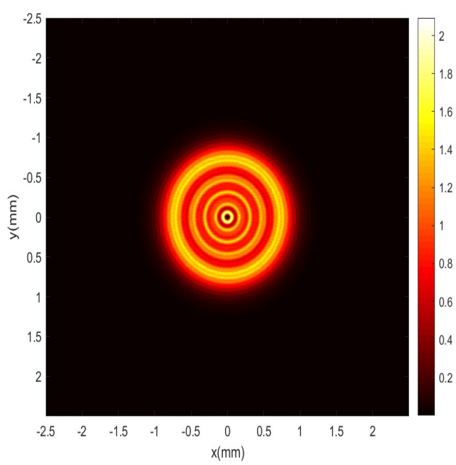

Fig. 10: Intensity pattern at d= 0.2m; s= 0.5

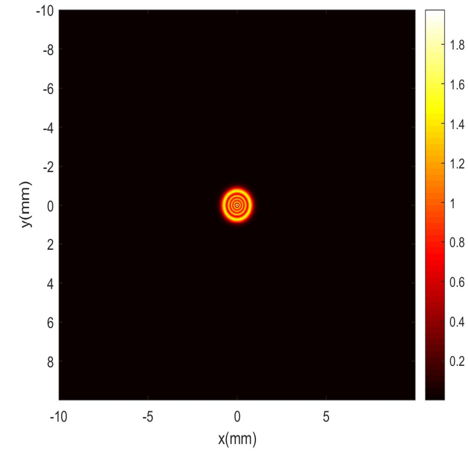

Fig. 11: Intensity pattern at d= 0.2m; s= 2

VI. Conclusion

In this paper, a comprehensive of diffraction theory and associated numerical techniques were discussed. The techniques were illustrated for both transparent and opaque objects. The techniques to address key issues such as intensity scaling, observation grid spacing, sampling requirement to satisfy nyquist criteria were discussed. It was shown that Angular spectrum method can be used for near-field applications and Fourier 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] P. H. Roberts, "A wave optics propagation code," Tech. Rep. TR-760, the Optical Sciences Company (1986).

[3] Alan V. Oppenheim and Ronald W. Schafer, Discrete-Time Signal Processing 2nd Edition (Prentice Hall: Upper Saddle River, NJ, 1999).

[4] C. Rydberg and J. Bengtsson, "Efficient numerical representation of the optical field for the propagation of partially coherent radiation with a specified spatial and temporal coherence function," J. Opt. Soc. Am. A 23(7), pp. 1616– 1625 (2006)

[5] S. Zablera, P. Cloetens, J.-P. Guigay, and J. Baruchel, "Optimization of phase contrast imaging using hard x rays", Review of Scientific Instruments 76, 073705 (2005);

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

[7] Hecht, Eugene. Optics. Reading, Mass: Addison-Wesley, 2002. Print.

[8] S. Coy, "Choosing mesh spacings and mesh dimensions for wave optics simulation," Proc. SPIE 5894, (2005).

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

[10] 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).