Fresnel diffraction from an aperture - Simpson's rule

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1. PROBLEM (A)

1.1 Problem

Simpson's Rule, accredited to the mathematician Thomas Simpson,^[1] is one of the many methods of approximation for numerical integration in numerical analysis. Practically, these methods of approximation are useful as they allow a numerical integral to be performed on many well-behaved functions that otherwise could not be integrated analytically. Consider a function which is composed of an integral:

$$f(t) = \int_0^t e^{-x^2} \mathrm{dx} \tag{1}$$

while f(t) is a fine function itself and though f(t) exists as an antiderivative of e^{-x^2} , it cannot however be expressed in $\operatorname{closed} \operatorname{form}$ i.e a composite of many elementary functions and thus cannot be integrated analytically. f(t) can only exists as a numerical value providing that t is one too. Here f(t) is an example of many nonelementary antiderivatives which has been proven to exist^[2] which can now be integrated by using Simpson's Rule to a degree of accuracy that depends on the computation time.

In short, the composite Simpson's Rule states that:

$$\begin{split} \int_{x_0}^{x_N} f(x) \mathrm{d}\mathbf{x} &\approx \frac{h}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + \\ & 2f_4 + \ldots + 2f_{N-2} + 4f_{N-1} + f_N) \\ & + O(h^5) \\ & \text{where } h = \frac{x_N - x_0}{N} \end{split} \tag{2}$$

where x_N and x_0 are the upper and lower limits of the integration respectively and N is the number of intervals for the integration. The task for part (a) was to write a function to perform Simpson's rule integration. The parameters taken as arguments by the functions and description on how to run the code by command line for part (a) are shown on table I and below. To perform integration of $\sin(x)$ from 0 to π using Simpson's Rule with N=20:

python $dn16018_ex2_code.py$ a -1 0 -u pi -n 20 -f sin

Likewise, for integration of cos(x) and e^x :

python $dn16018_ex2_code.py$ a -l 0 -u pi -n 20 -f cos

Flag	Arguments Description	Default Value
-1	Lower limit of integration	N/A
-u	Upper limit of integration	N/A
-n	Number of iterations (N)	N/A
-f	Type of function: sin, cos. exp	N/A

TABLE I.: The arguments that are taken by the Simpson's Rule function in part(a)

python dn16018_ex2_code.py **a -l 0 -u pi -n 20 -f** exp

Note: For Spyder, just use the bold part for command line options value.

1.2 Results

Part (a) aims to compare the approximated value of an integral for different values of N with its true value. The true value of the integral of $\sin(x)$ between π and 0 is given by:

$$\int_0^{\pi} \sin(x) \mathrm{d}x = 2$$

By using the same parameters with the same function on Simpson's Rule for say a value N of 10, this would be:

$$\int_0^{\pi} \sin(x) dx \approx \frac{\pi}{30} (f(0) + 4f(0.314...) + 2f(0.628...) + 4f(0.942...) + 2f(1.256...) + ... + 4f(2.827...) + f(\pi)) + O\left(\frac{\pi^2}{100}\right)$$
(3)

By taking the difference between the approximated value and true value of the integral, we can plot it against the interval of integration, N, to find out the rate of convergence of the approximated value towards the true value. A table of N up to 500 in increments of 50 and its corresponding value difference is shown on table II below.

It might look like form Fig. I that the approximated value is converging exponentially towards the true value of the integral. However, this is misleading due to the scaling of the graph since one can tell from Table II that there's a magnitude of 10 difference going from N = 50 to N = 100. Therefore, it

N	Value Difference
50	1.733×10^{-7}
100	1.082×10^{-8}
150	2.138×10^{-9}
200	6.765×10^{-10}
250	2.771×10^{-10}
300	1.336×10^{-10}
350	7.212×10^{-11}
400	4.228×10^{-11}
450	2.640×10^{-11}
500	1.732×10^{-11}

TABLE II.: The number of intervals for the Simpson's Rule and the difference between the approximated and true values.

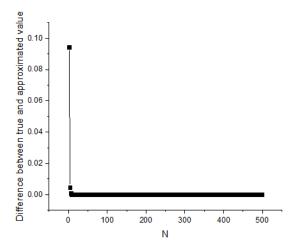


FIGURE 1 : The difference between the approximated value and true value against N.

would be more appropriate to plot Fig. 1 for a smaller interval of N to make the change apparent, or simply plot it as a logarithmic scale of base 10, both of which are shown on Fig. 2 and Fig. 3 below.

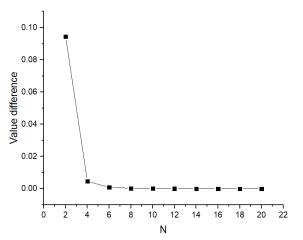


FIGURE 2 : A same graph as Fig. 2 but plotted over shorter interval of N.

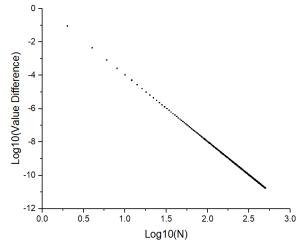


FIGURE 3: A logarithmic base 10 graph plotted for Fig. 1.

1.3 Discussion

It can be seen from Fig. 2 that starting from N = 8, the errors between the integrals become so insignificant that it is trivial to even compare it on the given scale. Retrospectively, this also implies that a large N the deviation of values are significant. At a very small value of error, a difference of a few magnitude do not give a significant meaning. Rather, it would be more interesting to see the rate of convergence of error towards 0 with respect to N. From Fig. 1 and Fig 2 it seems like the error is converging to 0 exponentially, however looking at the error change on Table II shows that those graphs are just a red-herring. A logarithmic base of 10 is chosen for Fig.3 since it's apparent from Fig. 2 and Table II that for N < 0, the value of error decreases at a magnitude of around 10. Fig. 3 is a much better representation of the rate of convergence of error, since the linear scale shows the absolute number error as N changes while the logarithmic scale shows the rate of decrease of error with respect to N, which is constant.

In fact, the remainder term for the Simpson's rule can be expressed as:^[3]

$$E = -\frac{(x_N - x_0)^5}{180N^5} f^{(4)}(\xi)$$
where $x_0 < \xi < x_N$ (4)

It can already be seen that for large N, Simpson's rule will compute the approximation of an integral to a very high degree of accuracy. Therefore it is worth investigating how the closeness of the integration limits affect the convergence rate of error. The same integral was computed between the limits of 0 and 1 and the results are shown below.

From Table III, it can be seen that the error of the Simpson's rule evaluation on the integral for the limits of 0 and 1 already has a really small value at as early as N=2. This confirms the validity of the equation 4, since N can only be an even whole integer and the smallest N can be is 2, so for $x_N-x_0<<2$, the error would have already been a small

N	Value Difference
2	1.645×10^{-4}
4	1.005×10^{-5}
6	1.977×10^{-6}
8	6.247×10^{-7}
10	2.557×10^{-7}
12	1.233×10^{-7}
14	6.652×10^{-8}
16	3.899×10^{-8}
18	2.434×10^{-8}
20	1.597×10^{-8}

TABLE III. : The number of intervals for the Simpson's Rule, $2 \le N \le 20$, and the difference between the approximated and true values for the integral of $\sin(x)$ between 0 and 1.

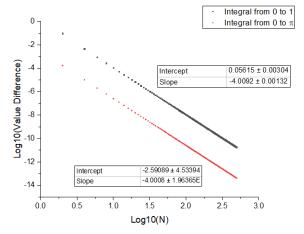


FIGURE 4: A logarithmic base 10 plot of error against N for integrals between limits of 0 to 1 and 0 to π using Simpson's rule.

value at small N(s) due to the fifth power in the equation. This also explains how Fig. 2 showed that the error is only at the same magnitude of value at around N=8, as π is comparably bigger than 2.

Surprisingly, the rate of convergence of error to 0 with respect to N does not change with the decreasing limit; it simply shifts the graph while maintaining the gradient, as shown in Fig. 4. It was shown that the higher the number of intervals for the integration, the more accurate the evaluation of a function between two limits using Simpson's rule will be, and that the analytical integration of a definite integral can just be modelled as performing Simpson's Rule on the same definite integral, taking the limit of $N \to \infty$. Ultimately, it was shown that for sufficient N, the error of an evaluation of a definite integral eventually become insignificant, if it were to model a real life scenario.

2. PROBLEM (B)

2.1 The problem.

Part (b) involves tweaking the Simpson's Rule function from part (a) so that an exponential function can be used within it. A couple more parameters were added into the function so that a single slit diffraction pattern can be produced across the x-axis of the screen, given by the equation:

$$X(x, y', z) = \int_{x'_1(y')}^{x'_2(y')} \exp\left[\frac{ik}{2z}(x - x')^2\right] dx' \qquad (5)$$

where i is the imaginary number, $k=2\pi/\lambda$, λ is the wavelength of light and z is the distance between the aperture and the screen. At each point x on the screen, an intensity of X(x,y',z) is evaluated by the Simpson's rule. The parameters taken as arguments by the functions and description on how to run the code by command line for part (b) are shown on table IV and below.

Flag	Arguments Description	Default Value
-Z	Distance between aperture and screen	1E-1
-n	Intervals of Integration(N)	50
-р	Number of points	100
-w	Wavelength	500E-9

TABLE IV.: The arguments that are taken by the Intensity function along the x-direction in part (b)

To run Part (b) with default value:

To run Part B with custom values (z = 1E-2m, N = 200, Number of Points = 300, Wavelength = 600nm):

Note: For Spyder, just use the bold part for command line options value.

2.2 Results

A Fraunhofer(far-field) and a Fresnel(close-field) diffraction pattern was successfully computed for the values of parameter listed in table V and table VI below using equation 5 and shown on Fig. 5 and Fig. 6 respectively.

2.3 Discussion

The diffraction pattern was obtained through repeatedly feeding different values of parameter by trial and error. It was known that Fraunhofer diffraction patterns are generated at a

Parameters Description	Values Used
Distance between aperture and screen	0.1m
Intervals of Integration(N)	50
Number of points	100
Wavelength	500E-9m
Screen Size x_{\min}	-5E-3m
Screen Size x_{max}	5E-3m
Aperture Size $x'_{\text{max}}, y'_{\text{max}}$	1E-5m
Aperture Size y'_{\min} , y'_{\min}	1E-5m

TABLE V. : The parameters used to generate the Fraunhofer diffraction pattern with a square aperture.

Parameters Description	Values Used
Distance between aperture and screen	0.0007m
Intervals of Integration(N)	50
Number of points	150
Wavelength	1400E-9m
Screen Size x_{\min}	-1.5E-4m
Screen Size x_{max}	1.5E-4m
Aperture Size x'_{max} , y'_{max}	9E-5m
Aperture Size y'_{\min} , y'_{\min}	-9E-5m

TABLE VI.: The parameters used to generate the Fresnel diffraction pattern with a square aperture.

far field so searching for the right distance at around the range of $0.05m \leqslant z \leqslant 0.5m$ was a reasonable decision. While investigating the value of z, it was also known again due to Fraunhofer diffraction being a far field one implies that the screen size will also be in around the same range of values as z. The same logic was applied to finding the Fresnel diffraction pattern.

For a fixed value of parameters with increasing N it can be seen that the plots get increasingly sharper and more defined. It seems to have less disturbances and small little sharp edges. This may be due to the fact that as N increases, the intensity evaluated at each point x on the screen becomes more accurate as its error becomes smaller. For constant values of parameters with varying z, it can be seen that the scale for which intensity spans increases as z is increased. It also showed that the plots fluctuates very chaotically. A logical explanation could be that when z is really small, a diffraction pattern can't be form due to how z is significantly small and comparable to the wavelength of light, therefore maximas and minimas could not happen.

3. PROBLEM (C)

3.1 The problem.

The same Simpson's Rule from part (B) is used to evaluate the same intensity for the y-coordinates on the screen. The electric field of the diffracted light at coordinates (x,y) at a distance z between the aperture and the screen is then found

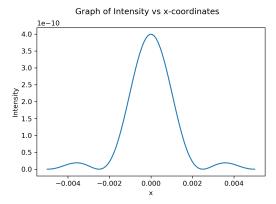


FIGURE 5: A 1-D Fraunhofer(far-field) diffraction pattern for z = 100mm

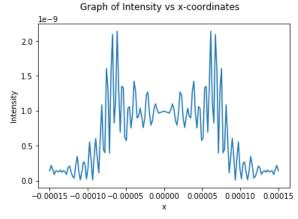


FIGURE 6: A 1-D Fresnel(close-field) diffraction pattern for z = 0.7mm

by multiplying both of the integral in each dimension, given by the equation:

$$E(x, y, z) = \frac{kE_0}{2\pi z} \int_{y_1'}^{y_2'} X(x, y', z) \exp\left[\frac{ik}{2z} (y - y')^2\right] dy'$$
(6)

The intensity of the diffraction pattern is then given by:

$$I(x, y, z) = \epsilon_0 c E(x, y, z) E^*(x, y, z)$$
(7)

where E^* is the complex conjugate of E, ϵ_0 is the permittivity of free space and c is the speed of light. A heat map of Intensity against x and y coordinates was then plotted. The parameters taken as arguments by the functions and description on how to run the code by command line for part (c) are shown on table V and below. To run Part (c)

- Square aperture with default value:
 python dn16018_ex2_code.py c-s square
- Square aperture with custom values(z = 1E-2m, N = 200, Number of Points = 300, Wavelength = 600nm)

Flag	Arguments Description	Default Value
-z	Distance between aperture and screen	1E-1
-n	Intervals of Integration(N)	50
-p	Number of points	100
-w	Wavelength	500E-9
-s	Aperture shape: square, circular, triangular	square
-y	Height	2E-4
-r	Radius	10E-5

TABLE VII. : The arguments that are taken by the Intensity function along the x-direction in part (b)

python dn16018_ex2_code.py **c -s square -z 1e-2 - n 200 -p 300 -w 600e-9**

- Circular aperture with default value:
 python dn16018_ex2_code.py c-s circular
- Circular aperture with custom values(z = 1E-2, N = 200, Number of points = 300, Wavelength = 600nm, radius = 10E-4):

python dn16018_ex2_code.py **c -s circular -z 1e-2** -n 200 -p 300 -w 600e-9 -r 10e-4

- Triangular aperture with default value:
 python dn16018_ex2_code.py c-striangular
- Triangular aperture with custom values(z = 1E-2, N = 200, Number of points = 300, Wavelength = 600nm, ymax = 2E-3):

python dn16018_ex2_code.py **c-s triangular -z 1e-2 -n 200 -p 300 -w 600e-9 -r 10e-4 -y 2e-3**

Note: For Spyder, just use the bold part for command line options value.

3.2 Results

The diffraction patterns for different aperture and its values that were used to generate the plot are shown in the tables VII, VIII and IX below.

3.3 Discussion

Since the screen size for part (c) does not play a huge role in changing the image of the diffraction pattern, rather it only either enlarges or reduces the projection of the image onto the screen, so it was fixed to values where each of the image will fit exactly onto the screen for different aperture shapes of different z. The shape change of the aperture into triangular and circular were achieved by taking in one new parameter for

Parameters Description	Values Used
Distance between aperture and screen	$5\text{E-3m} \leqslant z \leqslant 25\text{E-3m}$
Intervals of Integration(N)	50
Number of points	200
Wavelength	500E-9m
Screen Size x_{max} , y_{max}	9E-5m
Screen Size y_{\min} , y_{\min}	-9E-5m
Aperture Size $x'_{\text{max}}, y'_{\text{max}}$	10E-5m
Aperture Size y'_{\min} , y'_{\min}	-10E-5m

TABLE VIII.: The parameters used to generate the diffraction pattern with a square aperture.

Graph of Intensity vs x and y coordinates

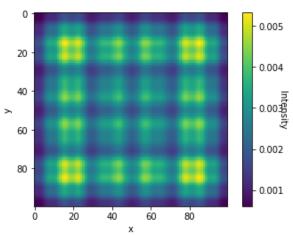


FIGURE 7: 2-D diffraction pattern through a square aperture for z = 5mm

Parameters Description	Values Used
Distance between aperture and scre	en 5E-3m $\leqslant z \leqslant$ 25E-3m
Intervals of Integration(N)	50
Number of points	200
Wavelength	500E-9m
Screen Size x_{max} , y_{max}	9E-5m
Screen Size y_{\min} , y_{\min}	-9E-5m
Aperture Radius	10E-5m

TABLE IX. : The parameters used to generate the diffraction pattern with a circular aperture.

Parameters Description	Values Used
Distance between aperture and screen	5E-3m≤ <i>z</i> ≤25E-3m
Intervals of Integration(N)	100
Number of points	50
Wavelength	500E-9m
Screen Size $x_{\text{max}}, y_{\text{max}}$	17E-5m
Screen Size y_{\min} , y_{\min}	-17E-5m
Triangular Aperture Height	2E-4m

TABLE X.: The parameters used to generate the diffraction pattern with a triangular aperture.

each shape, radius for the circular aperture and height for the

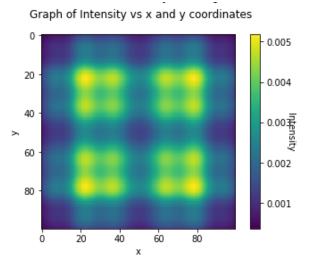


FIGURE 8: 2-D diffraction pattern through a square aperture for z = 10mm

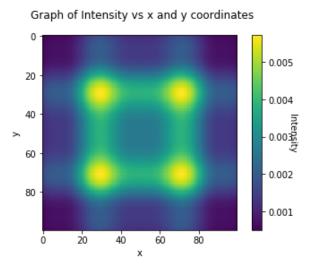


FIGURE 9: 2-D diffraction pattern through a square aperture for z = 15mm

triangular aperture. By using the equation of circle and some trigonometric equation involving an equilateral triangle, one can set up a loop such that for every loop the double integral is being evaluated then summed, with a series of ever-changing upper and lower limits in both x and y direction.

It was worth investigating whether if there exists a value of N whereby the error computed by the Simpson's Rule is so small that the image no longer have any significant differences should N increase even more. The diffraction through the square aperture was used for this investigation as it takes the shortest amount of time to compute out of the three. For the same parameter values, which are z=5mm, number of points = 100, wavelength = 500nm, aperture sizes of $\pm 10E-5$ m either side and a screen size of $\pm 9E-5$ m, each graph is plotted with a increasing values of N by increments of 10 from 10 to 120 and made into a .gif image online. [4] It can be seen from the .gif image that at N=40, the effect of increasing N

Graph of Intensity vs x and y coordinates

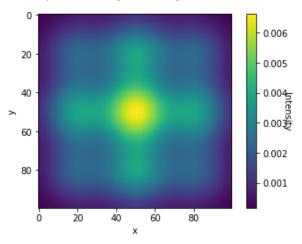


FIGURE 10: 2-D diffraction pattern through a square aperture for z = 20mm

Graph of Intensity vs x and y coordinates

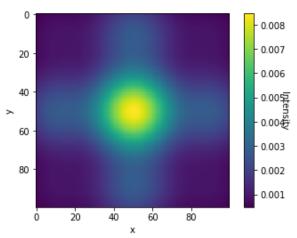


FIGURE 11: 2-D diffraction pattern through a square aperture for z = 25mm

even further becomes trivial. The same .gif image was also created [5] for $z=30\mathrm{mm}$ and with increasing N. The same thing starts to happen at N=8 where the human eyes can no longer perceive the difference between the image at N=8 and N=10.

REFERENCES

- [1] O'Connor, J. J. and Robertson, E. F. "Thomas Simpson." Mac-Tutor History of Mathematics. JOC/EFR, 1996. http://wwwgroups.dcs.stand.ac.uk/ history/Mathematicians/Simpsons.html
- [2] Dunham. W (2005), The Calculus Gallery. Princeton. p. 119.
- [3] P. J. Davis, W. Rheinbolt, P. Rabinowitz (2014), *Methods of Numerical Integration*. Academic Press. p. 20-21.
- [4] D. Ng. https://giphy.com/gifs/xThtaxyzJvYc72pjdm
- [5] D. Ng. https://giphy.com/gifs/3o7WILTL2oWX704DDO

Graph of Intensity vs x and y coordinates

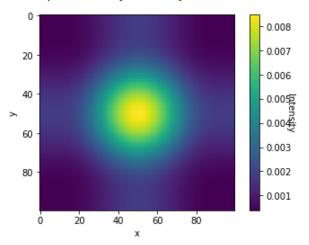


FIGURE 12: 2-D diffraction pattern through a square aperture for z = 30mm

Graph of Intensity vs x and y coordinates

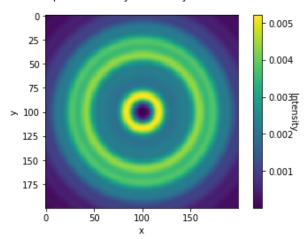


FIGURE 13: 2-D diffraction pattern through a circular aperture for z = 5 mm

Graph of Intensity vs x and y coordinates

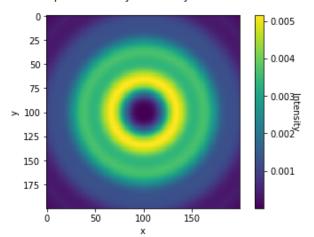


FIGURE 14: 2-D diffraction pattern through a circular aperture for z = 10 mm

Graph of Intensity vs x and y coordinates

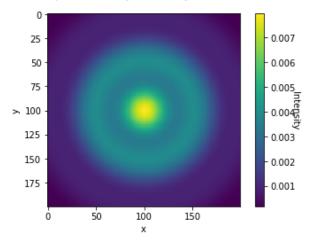


FIGURE 15: 2-D diffraction pattern through a circular aperture for z = 15 mm

Graph of Intensity vs x and y coordinates

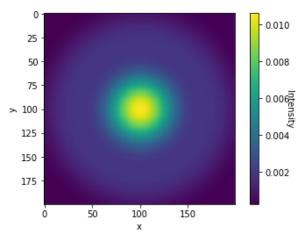


FIGURE 16: 2-D diffraction pattern through a circular aperture for z = 20mm

Graph of Intensity vs x and y coordinates

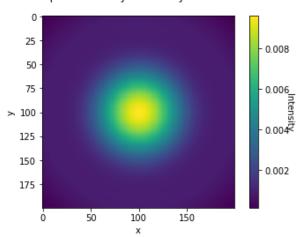


FIGURE 17: 2-D diffraction pattern through a circular aperture for z = 25 mm

Graph of Intensity vs x and y coordinates

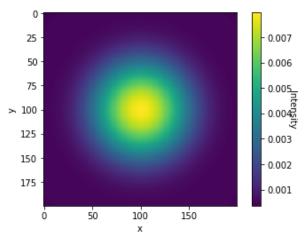


FIGURE 18: 2-D diffraction pattern through a circular aperture for z = 30 mm

Graph of Intensity vs x and y coordinates

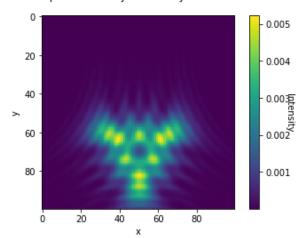


FIGURE 19: 2-D diffraction pattern through a triangular aperture for z = 5 mm

Graph of Intensity vs x and y coordinates

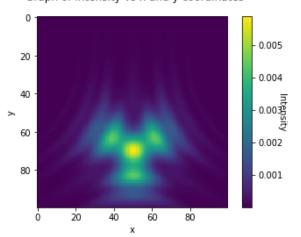


FIGURE 20: 2-D diffraction pattern through a triangular aperture for z = 10 mm

Graph of Intensity vs x and y coordinates

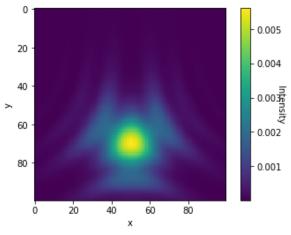


FIGURE 21: 2-D diffraction pattern through a triangular aperture for z = 15 mm

Graph of Intensity vs x and y coordinates

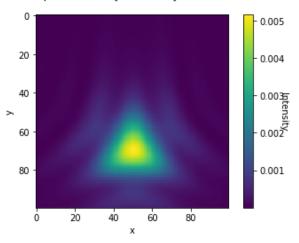


FIGURE 22: 2-D diffraction pattern through a triangular aperture for z = 20mm

Graph of Intensity vs x and y coordinates

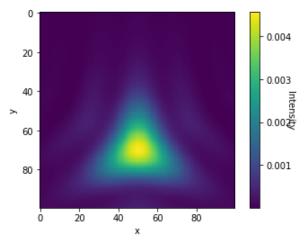


FIGURE 23: 2-D diffraction pattern through a triangular aperture for z = 25 mm

Graph of Intensity vs x and y coordinates

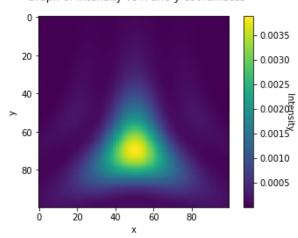


FIGURE 24: 2-D diffraction pattern through a triangular aperture for z = 30 mm