Numerical Integration

HW 2: Wednesday, Sep. 11, 2019
DUE: Wednesday, Sep. 18, 2019
READ: Numerical Recipes in C++, section 4.0-4.4 pages 155-172
(optional: section 4.6, 7,8 pages 179-200)
OPTIONAL: Landau, Paez, and Bordeianu, integration, section 6.0 to 6.4

You should continue reading the book you have chosen on C/C++ programming.

PROBLEM:

Fresnel diffraction theory describes the diffraction of electromagnetic waves (in this problem, light waves) in the near field (i.e. a distance small compared to the size of the diffracting object and/or the wavelength of the waves). When light waves are incident upon a straight edge that is opaque for $x < 0$ and nonexistent for $x > 0$ (see Figure 1) the light waves near the edge ($x_0 = 0$) interfere in interesting ways.

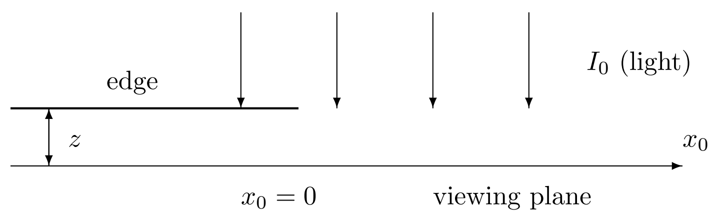

Figure 1: Fresnel near-field diffraction of light near an edge.

The analytical Fresnel diffraction theory comes to a halt when the following integral is reached:

$$\begin{aligned} I(x_0) &= \text{const.} \times \left| \int_0^{+\infty} \exp\left[\frac{i\pi}{\lambda z}(x_0 - x)^2 \right] dx \right|^2 \\ &= \frac{I_0}{\lambda z} \left| \int_{-\infty}^{x_0} \exp\left(\frac{i\pi x^2}{\lambda z} \right) dx \right|^2 \end{aligned} \tag{1}$$

where I_0 is the incident intensity, λ is the wavelength of the light, z is the distance between the edge and the viewing screen, and x_0 is the position in the viewing plane.

This integral describes the intensity of light $I(x_0)$ in the viewing plane, at a distance x_0 from the edge. It results from adding all waves with the appropriate path length, assuming small angles. The goal here is to evaluate this integral. Although you do not need to be concerned with the analytical theory used to derive this expression, you may refer to Section 13.1 of Heald and Marion[2] (or any of several other optics textbooks) for more details if you are interested.

The goal of this homework is to numerically evaluate the integral I/I_0 for z=1.0 micron, and a wavelength of λ=0.5 microns (green light). (It is interesting to note that this is roughly the size of a transistor so that this effect might be relevant for optoelectronic devices or optical nano-lithography.)

This integral is not very well behaved. The integrand oscillates wildly and the limits go to infinity. It is better to rearrange it in terms of the so-called Fresnel integrals $S(u)$ and $C(u)$ and a dimensionless parameter u_0:

$$I(u_0) = \frac{1}{2} I_0 \left\{ [C(u_0) - C(-\infty)]^2 + [S(u_0) - S(-\infty)]^2 \right\} \tag{2}$$

$$C(u_0) = \int_0^{u_0} \cos\left(\frac{\pi}{2} u^2\right) du \tag{3}$$

$$S(u_0) = \int_0^{u_0} \sin\left(\frac{\pi}{2} u^2\right) du \tag{4}$$

$$u_0 = x_0 \sqrt{\frac{2}{\lambda z}} \tag{5}$$

$$C(-\infty) = S(-\infty) = -0.5 \tag{6}$$

The integrand is still not well behaved (i.e. oscillating) but the limits are now reasonable.

First write a program that calculates $I(u_0 = 0.5)/I_0$ and $I(u_0 = 3)/I_0$ for $n = 4, 8, 16, 32, \ldots, 8192$ points using the trapezoid rule. You should include a short table in your write-up. It is best to write a single function that returns $I(u_0)/I_0$ as a function of u_0 and n. You might also want to make two more functions (one each for $C(u)$ and $S(u)$).

Next choose a value of n to give at least 4 or 5 significant digits and produce a file with about 200 points between $x_0 = -1$ microns and $x_0 = +4$ microns. Plot I/I_0 in this range. Compare this graph to your expected values for large and small x_0 and any other relevant physical characteristics.

(The value $I(x_0 = 0) = 0.25 I_0$ is one of the few values that can be calculated analytically.)

OPTIONAL: Try automating the search for a proper number of points (using the Trapezoid rule or Simpson's rule, as in section 4.2 of Numerical Recipes[3]) for the final graph.

NOTE-1: The $S(u)$ and $C(u)$ integrals are tabulated in chapter 7 of Abramowitz and Stegun[1]

NOTE-2: In C/C++ the value of π can be found from: `pi = 4.0 * atan( 1.0 );`

NOTE-3: In C++ streams, if fp is an ofstream, the following may be used to change the number of output digits:

```
fp.precision(9);   // select 9 digits
```

References

[1] M. Abramowitz and I. A. Stegun, editors, *Handbook of Mathematical Functions*, National Bureau of Standards, 1964, and Dover 1965.

[2] M. A.Heald and J. B. Marion, *Classical Electromagnetic Radiation (3rd edit.)*, Saunders 1995, Section 13.1.

[3] W. H. Press, S. A, Teukolsky, W. T. Vetterling and B. P. Flannery *Numerical Recipes, The Art of Scientific Computing, 3rd edit.*, Camb. Univ. Press 2007.

An efficient recursive form of the trapezoid rule in algorithmic form, to a tolerance of tol is:

$n \leftarrow 1$ (number of intervals NOT points)
$S \leftarrow 0.5[f(x_{min}) + f(x_{max})]$
$I_{NEW} \leftarrow (x_{max} - x_{min}) \times S$
repeat
    $n \leftarrow 2n$
    $\Delta x \leftarrow (x_{max} - x_{min})/n$
    $I_{OLD} \leftarrow I_{NEW}$
    $S \leftarrow S + \sum_{i=1,3,5,\cdots,(n-1)} f(x_{min} + i\Delta x)$
    $I_{NEW} \leftarrow S\Delta x$
until $|I_{NEW} - I_{OLD}| < |tol|$ and $n > n_{min} \sim 8$
I_{NEW} is the integral

An efficient recursive form of Simpson's rule in algorithmic form, to a tolerance of tol is:

$n \leftarrow 2$ (number of intervals NOT points)
$S_1 \leftarrow f(x_{min}) + f(x_{max})$
$S_2 \leftarrow 0$
$S_4 \leftarrow f(\frac{1}{2}(x_{min} + x_{max}))$
$I_{NEW} \leftarrow 0.5(x_{max} - x_{min})(S_1 + 4S_4)/3$
repeat
    $n \leftarrow 2n$
    $\Delta x \leftarrow (x_{max} - x_{min})/n$
    $S_2 \leftarrow S_2 + S_4$
    $I_{OLD} \leftarrow I_{NEW}$
    $S_4 \leftarrow \sum_{i=1,3,5,\cdots,(n-1)} f(x_{min} + i\Delta x)$
    $I_{NEW} \leftarrow \Delta x(S_1 + 2S_2 + 4S_4)/3$
until $|I_{NEW} - I_{OLD}| < |tol|$ and $n > n_{min} \sim 8$
I_{NEW} is the integral