Exact Finite Difference Schemes for Solving Helmholtz Equation at Any Wavenumber: reproducing the results

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Purpose

Reproduce the results of the publication [1]. The ultimate purpose being to use this method to our problem: the computation of the Helmholtz equation:

$$\begin{cases} \nabla^2 u + k^2 u = 0, x\epsilon[a,b] \\ \dfrac{\partial u}{\partial n} = iku\ (Sommerfeld) \\ U(a) = \alpha\ (Dirichlet) \end{cases} \tag{1}$$

Here $k = \frac{\omega}{c} = \frac{2\pi}{cT} = 2\pi f = 2\pi/\lambda$ (c: the celerity of the wave, T: the period, f: the frequency, λ: the wave length).

For sake of pedagogical purpose, we want to reproduce the new algorithm method for the one dimensional problem and the two dimensional problem exposed in the work of [1] and compare it with the ancient scheme. The latter is not explicitly given for what concerns the boundary and especially how to apply the Sommerfeld condition and has been rebuilt thanks to the explanation given in [2]. A pedagogical explanation about the general scheme matrix building process may be found in [3] and [4].

Protocol

The computation of the Helmholtz equation is done for the one dimensional and the two dimensional problem.
Two different schemes are available for the computation of the interior points: the classical 3 (1 dimension) and 5 (2 dimension) schemes and the new version of this scheme.
Three different schemes are available for the computation of the boundary points: Dirichlet boundary, the Sommerfeld condition with classical central difference and the Sommerfeld condition with the new difference scheme.

The one dimensional problem

The following equations are valid for the one-dimensional problem.

$$\begin{cases} \nabla^2 u(x) + k^2 u(x) = 0, x\epsilon[a,b] \\ \dfrac{\partial u(x)}{\partial x} = iku(x)\ (Sommerfeld) \\ U(a) = \alpha\ (Dirichlet) \end{cases} \tag{2}$$

The following schemes may be calculated from the second order Taylor series. For a demonstration of each of these, see One dimensional problem in Appendices.

Standard Scheme

The classical algorithm is composed of four schemes. These provide the coefficients that are given to the elements of the scheme matrix A and, in case of Dirichlet constraint, of the vector b. The step chosen for the discretization is h. If just k is given, h may be calculated such that $kh \sim 0.5$ from [1].

Points type	Scheme
Interior	$[2-(kh)^2]u_i - u_{i+1} - u_{i-1} = 0$

Dirichlet[1]	$b(i) = \alpha$
Sommerfeld (right)	$[2-(kh)^2-2ikh]u_i - 2u_{i-1} = 0$
Sommerfeld (left)	$[2-(kh)^2+2ikh]u_i - 2u_{i+1} = 0$

Table 1. One dimensional standard schemes

New scheme

The classical algorithm is composed of four schemes. These give the coefficients that are given to the elements of the scheme matrix A and, in case of Dirichlet constraint, of the vector b.

The general schemes that are given by [1] are recalled hereunder. It allows us to directly derive a practical expression of the scheme for the central point and the extremity (left and right) governed by Sommerfeld constraint.

$$\begin{cases} -k^2u_i = \dfrac{1}{h^2}[u_{i+1} - \omega u_i + u_{i-1}] \\ \omega = 2\cos(kh) + (kh)^2 \\ u_{i+1} - 2i\sin(kh)u_i - u_{i-1} = 0 \end{cases} \tag{3}$$

Points type	Scheme
Interior	$2\cos(kh)u_i - u_{i+1} - u_{i-1} = 0$
Dirichlet	$b(i) = \alpha$
Sommerfeld (right)	$2[\cos(kh) - i\sin(kh)]u_i - 2u_{i-1} = 0$
Sommerfeld (left)	$2[\cos(kh) + i\sin(kh)]u_i - 2u_{i+1} = 0$

Table 2. One dimensional new schemes

The two dimensional problem

The following equations are valid for the one-dimensional problem.

$$\begin{cases} \nabla^2 u(x,y) + k^2u(x,y) = 0, x\epsilon[a,b] \\ \dfrac{\partial u(x,y)}{\partial n} = iku(x,y)\ (Sommerfeld) \\ u(x,y) = \alpha\ (Dirichlet) \end{cases} \tag{4}$$

The following schemes may be calculated from the second order Taylor series. The vector n is the unit vector normal to the region. We purposely do not detail too much the Dirichlet condition for it may be a source point, a segment of a side, a combination of sides of the region. What is sure is the Sommerfeld may not be applied to the entire region. For a demonstration of each of these, see Two dimensional problem in Appendices.

Standard scheme

The classical algorithm is composed of 10 schemes that are detailed hereunder. Two times four schemes are devoted to the differences between the Sommerfeld constraint applied for each of the side (north, east, south, west) and the ones devoted to the differences

[1] The Dirichlet condition is applied by replacing the unknown point (also called the phantom point) by its known value i.e. its Dirichlet value. Thus the calculation of the rightmost point of the line (for the one dimensional problem) is given by $[2-(kh)^2]u_i - u_{i-1} = 0$ that gives the coefficient of the matrix and u_{i+1} that take the Dirichlet value α is placed in the vector b thus $b(i) = \alpha$ for more details about this technique see [4] or [3].

between the Sommerfeld constraint applied on the corner points (NE, SE, SW, NW). Because of the nature of the derivation (along the normal vector (2)) in the Sommerfeld constraint, the results is not directly obtained and is demonstrated later see Two dimensional problem in Appendices.

Points type	Scheme
Interior	$[4-(kh)^2]u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = 0$
Dirichlet	$b(l) = \alpha$
Sommerfeld (east boundary)	$[4-(kh)^2 - 2ikh]u_{i,j} - 2u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = 0$
Sommerfeld (west boundary)	$[4-(kh)^2 + 2ikh]u_{i,j} - 2u_{i+1,j} - u_{i,j+1} - u_{i,j-1} = 0$
Sommerfeld (north boundary)	$[4-(kh)^2 - 2ikh]u_{i,j} - u_{i+1,j} - u_{i-1,j} - 2u_{i,j-1} = 0$
Sommerfeld (south boundary)	$[4-(kh)^2 + 2ikh]u_{i,j} - u_{i+1,j} - u_{i-1,j} - 2u_{i,j+1} = 0$
Sommerfeld (north-east corner boundary)	$[2-\frac{1}{2}(kh)^2 - i\sqrt{2}kh]u_{i,j} - u_{i-1,j} - u_{i,j-1} = 0$
Sommerfeld (south-east corner boundary)	$[2-\frac{1}{2}(kh)^2 - i\sqrt{2}kh]u_{i,j} - u_{i-1,j} - u_{i,j+1} = 0$
Sommerfeld (south-west corner boundary)	$[2-\frac{1}{2}(kh)^2 - i\sqrt{2}kh]u_{i,j} - u_{i+1,j} - u_{i,j+1} = 0$
Sommerfeld (north-west corner boundary)	$[2-\frac{1}{2}(kh)^2 - i\sqrt{2}kh]u_{i,j} - u_{i+1,j} - u_{i,j-1} = 0$

Table 3. Two dimensional standard schemes

New scheme

In order to build the new schemes that mirror what has been done in the preceding paragraph, we have the following description of the problem:

$$\begin{cases} \nabla^2 u + k^2 u = 0 \\ \dfrac{\partial u}{\partial x} = ik_1 u \ (Sommerfeld) \\ \dfrac{\partial u}{\partial y} = ik_2 u \ (Sommerfeld) \\ u(x,y) = \alpha \ (Dirichlet) \end{cases} \tag{5}$$

The general schemes that are given by [1] are recalled here:

$$\begin{cases} 4J_0(kh)u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = 0, & i,j \in [1,n] \\ u_{n+1,j} - 2isin(k_1 h)u_{n,j} - u_{n-1,j} = 0, & j \in [1,n] \\ u_{j,n+1} - 2isin(k_2 h)u_{n,j} - u_{j,n-1} = 0, & j \in [1,n] \end{cases} \tag{6}$$

The parameter J_0 is the Bessel function defined by: $J_0(kh) = \frac{1}{\pi}\int_0^{\pi} \cos(khsin(\theta))\, d\theta$ and is currently available on mathematical calculation platform. The parameter θ is in general not available and has to be chosen arbitrarily for each calculation. The following table sums up the practical schemes that may be almost directly deduced from (6).

Points type	Scheme
Interior	$[4J_0(kh)u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = 0$
Dirichlet	$b(l) = \alpha$
Sommerfeld (east boundary)	$[4J_0(kh) - 2isin(k_1h)]u_{i,j} - 2u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = 0$
Sommerfeld (west boundary)	$[4J_0(kh) + 2isin(k_1h)]u_{i,j} - 2u_{i+1,j} - u_{i,j+1} - u_{i,j-1} = 0$
Sommerfeld (north boundary)	$[4J_0(kh) - 2isin(k_2h)]u_{i,j} - u_{i+1,j} - u_{i-1,j} - 2u_{i,j-1} = 0$
Sommerfeld (south boundary)	$[4J_0(kh) + 2isin(k_2h)]u_{i,j} - u_{i+1,j} - u_{i-1,j} - 2u_{i,j+1} = 0$
Sommerfeld (north-east corner boundary)	$[4J_0(kh) - 2isin(k_1h) - 2isin(k_2h)]u_{i,j} - 2u_{i-1,j} - 2u_{i,j-1} = 0$
Sommerfeld (south-east corner boundary)	$[4J_0(kh) - 2isin(k_1h) + 2isin(k_2h)]u_{i,j} - 2u_{i-1,j} - 2u_{i,j+1} = 0$
Sommerfeld (south-west corner boundary)	$[4J_0(kh) + 2isin(k_1h) + 2isin(k_2h)]u_{i,j} - 2u_{i+1,j} - 2u_{i,j+1} = 0$
Sommerfeld (north-west corner boundary)	$[4J_0(kh) + 2isin(k_1h) - 2isin(k_2h)]u_{i,j} - 2u_{i+1,j} - 2u_{i,j-1} = 0$

Table 4. Two dimensional new schemes

Results

Appendices

Taylor expansions

During the following demonstration we use different version of the Taylor expansion. They are grouped here:

$$u(\mathrm{x}+\mathrm{h}) = u(x) + u^{(1)}(x)h + \frac{1}{2}u^{(2)}(x)h^2 + \frac{1}{6}u^{(3)}(a)h^3 + O(h^4) \quad (7)$$

$$u(\mathrm{x}-\mathrm{h}) = u(x) - u^{(1)}(x)h + \frac{1}{2}u^{(2)}(x)h^2 - \frac{1}{6}u^{(3)}(a)h^3 + O(h^4) \quad (8)$$

One dimensional problem

Standard scheme

Interior point

By adding (7) and (8) we obtain the central difference:

$$\frac{1}{h^2}[u(\mathrm{x}-\mathrm{h}) - 2u(x) + u(\mathrm{x}+\mathrm{h})] = u^{(2)}(x) + O(h^2)$$

And from equation (2) we may build the scheme:

$$\frac{1}{h^2}[u_{i-1} - 2u_i + u_{i+1}] + k^2u_i = 0$$

That gives directly the interior point scheme:

$$[2-(kh)^2]u_i - u_{i+1} - u_{i-1} = 0 \tag{9}$$

Sommerfeld point

By subtracting (8) from (7) we obtain the following approximation that is called the central scheme for the first order derivative:

$$u(\mathrm{x}+\mathrm{h}) - u(\mathrm{x}-\mathrm{h}) = 2hu^{(1)}(x) + O(h^3) \tag{10}$$

And the Sommerfeld constraint of (2) may therefore be written as:

$$\frac{\partial u}{\partial x} = \frac{1}{2h}[u(x+h) - u(x-h)] + O(h^2) = iku(x)$$

And this lead directly to the following scheme:

$$u_{i+1} - u_{i-1} = i2khu_i \tag{11}$$

Now if we want to build the Sommerfeld scheme for the rightmost point of the one dimensional line we may replace the new expression of $\mathrm{u}_{\mathrm{i}+1}$ from equation (11) in the central difference point (9). Alternatively, an expression of $\mathrm{u}_{\mathrm{i}-1}$ may be built from (11) and replace in equation (9) and this for the leftmost point. This lead directly to the scheme expression for Sommerfeld written in: Table 1.
For instance, the left extremity may be described this way:

$$\begin{cases} u_{i-1} = u_{i+1} - i2khu_i \\ [2-(kh)^2]u_i - u_{i+1} - u_{i-1} = 0 \end{cases}$$

That gives:

$$[2-(kh)^2 + i2khu_i]u_i - 2u_{i+1} = 0$$

Two dimensional problem

Standard scheme

Interior point

By the same process that we have obtained the central point scheme for the one dimensional problem we may write from the addition of the two equations (7) and (8) in their two dimensional version:

$$\begin{aligned}\frac{1}{h^2}[u(\mathrm{x}-\mathrm{h},\mathrm{y}) - 2u(x,y) + u(\mathrm{x}+\mathrm{h},\mathrm{y}) + u(\mathrm{x},\mathrm{y}-\mathrm{h}) - 2u(x,y) + u(\mathrm{x},\mathrm{y}+\mathrm{h})] \\ = u^{(2)}(x,y) + O(h^2)\end{aligned}$$

This gives us and expression for the second order derivative and we deduce the following central point scheme from equation (4):

$$\frac{1}{h^2}\left[-4u_{i,j} + u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right] + k^2 u_{i,j} = 0$$

And by multiplying each side by $-h^2$ we find the expression of Table 3.

$$[4 - (kh)^2]u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = 0 \tag{12}$$

Sommerfeld point

We recall that from equation (4) we have the following Sommerfeld condition: $\frac{\partial u(x,y)}{\partial n} = iku(x,y)$ with n being the normal unit vector to the region considered. In terms of scheme, which is what we are looking for, we may differentiate two types of points.

Side points

The first is the side points, for which the normal vector is simply the unit vector along the x axis for the east and west side of the region and the unit vector along the y axis for the north and south side of the region.
We will take the east side as a prototype for the demonstration and the other sides may be deduced the same way. The central scheme for the first order derivative along the x axis is given by (10) and from the Sommerfeld condition this may be equalized as:

$$\frac{1}{2h}[u(x+h,y) - u(x-h,y)] = iku(x,y)$$

This let us write the following scheme:

$$u_{i+1,j} - u_{i-1,j} = i2khu_{i,j} \tag{13}$$

Now suppose that we want to write a scheme for the east most point of our region. From the central scheme (12) we ignore the value of $u_{i+1,j}$ but we may now replace it by its new expression from (13) and obtain the scheme written for the east side in Table 3.
All the other side points are obtained by the same procedure.

Corner points

The second is the corner point for which the normal vector is the unit vector along the diagonal of the unit square.
We will take the north east corner as a prototype for our demonstration and the other corner scheme may be obtained the same way.
Our diagonal unit vector may be written: $n = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})$. Therefore the Sommerfeld condition may be written:

$$\frac{\partial u(x,y)}{\partial n} = \left(\frac{\partial u(x,y)}{\partial x}, \frac{\partial u(x,y)}{\partial y}\right).n = \left(\frac{\partial u(x,y)}{\partial x}, \frac{\partial u(x,y)}{\partial y}\right).(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}) = iku(x,y)$$

We then sum two version of equation (8) in its two dimensional version, one at constant y and the other at constant x and obtain:

$$\frac{\partial u(x,y)}{\partial x} + \frac{\partial u(x,y)}{\partial y} = \frac{1}{h}[2u(x,y) - u(x-h,y) - u(x,y-h) + \frac{h^2}{2}\left(\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2}\right)]$$

Now the Sommerfeld condition may be written:

$$\frac{\partial u(x,y)}{\partial n} = \frac{\sqrt{2}}{2h}[2u(x,y) - u(x-h,y) - u(x,y-h) + \frac{h^2}{2}\left(\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2}\right)] = iku(x,y)$$

And an expression for the second order derivative may be extracted:

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = \frac{2}{h^2}[\sqrt{2}ikhu(x,y) - 2u(x,y) + u(x-h,y) + u(x,y-h)]$$

And if we replace this second order derivative expression in (4) we obtain the scheme version of the Helmholtz equation:

$$\frac{2}{h^2}\left[\sqrt{2}ikhu_{i,j} - 2u_{i,j} + u_{i-1,j} + u_{i,j-1}\right] + k^2 u_{i,j} = 0$$

And the last equation let us find directly the scheme given in Table 3 for the north east point. The other corner points are obtain the same way but by starting with the appropriate combination of the version of the Taylor expansion as well as by noting that the diagonal unit vector may have changes in the sign of its coefficients.

Bibliography

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