Final Report

M.Sc Degree in Computer Science

Hadassah Academic College

Title: Frequency-dependent attenuation in fractional Helmholtz wave equations

[Final Report 1](#_Toc436559325)

[M.Sc Degree in Computer Science 1](#_Toc436559326)

[Hadassah Academic College 1](#_Toc436559327)

[Title: Frequency-dependent attenuation in fractional Helmholtz wave equations 1](#_Toc436559328)

[Abstract 6](#_Toc436559329)

[Presentation of the problem and definition of the objectives 8](#_Toc436559330)

[Background 9](#_Toc436559331)

[Ultrasound: general characteristics 9](#_Toc436559332)

[The physics of the problem 10](#_Toc436559333)

[Speed of sound and power law attenuation 10](#_Toc436559334)

[Fractional wave equations from time to frequency domain 11](#_Toc436559335)

[Frequency-dependent attenuation in the Helmholtz equations 12](#_Toc436559336)

[Boundary values 13](#_Toc436559337)

[Analysis of the problem 14](#_Toc436559338)

[General considerations 14](#_Toc436559339)

[Choice of the Helmholtz equation 14](#_Toc436559340)

[Choice of the numerical method 15](#_Toc436559341)

[Finite differences 16](#_Toc436559342)

[Finite elements 16](#_Toc436559343)

[Finite Volumes 18](#_Toc436559344)

[Spectral Methods 18](#_Toc436559345)

[Discussion 19](#_Toc436559346)

[The finite difference method (FDM) 20](#_Toc436559347)

[Introduction 20](#_Toc436559348)

[Basic Scheme for order 1 and 2 operators 21](#_Toc436559349)

[Derivatives 21](#_Toc436559350)

[Taylor Expansion 22](#_Toc436559351)

[Truncation Error 23](#_Toc436559352)

[Sin(x) example 24](#_Toc436559353)

[Discussion 25](#_Toc436559354)

[A first practical case: The Poisson Equation 26](#_Toc436559355)

[BVP 27](#_Toc436559356)

[Discussion 29](#_Toc436559357)

[Schemes for the Helmholtz Equation 29](#_Toc436559358)

[Presentation of the boundary value problem 30](#_Toc436559359)

[Classical scheme (2nd order) 31](#_Toc436559360)

[The two dimensional problem 31](#_Toc436559361)

[Standard scheme 31](#_Toc436559362)

[Exact Scheme 32](#_Toc436559363)

[Compact 4th and 6th order schemes 33](#_Toc436559364)

[*Order* 34](#_Toc436559365)

[34](#_Toc436559366)

[34](#_Toc436559367)

[34](#_Toc436559368)

[2nd 34](#_Toc436559369)

[34](#_Toc436559370)

[34](#_Toc436559371)

[34](#_Toc436559372)

[4th 34](#_Toc436559373)

[34](#_Toc436559374)

[34](#_Toc436559375)

[34](#_Toc436559376)

[6th 34](#_Toc436559377)

[34](#_Toc436559378)

[34](#_Toc436559379)

[34](#_Toc436559380)

[*Order* 35](#_Toc436559381)

[35](#_Toc436559382)

[35](#_Toc436559383)

[35](#_Toc436559384)

[2nd 35](#_Toc436559385)

[35](#_Toc436559386)

[35](#_Toc436559387)

[35](#_Toc436559388)

[6th 35](#_Toc436559389)

[35](#_Toc436559390)

[35](#_Toc436559391)

[35](#_Toc436559392)

[Architecture of the algorithm and code 35](#_Toc436559393)

[Choice of the technologies 35](#_Toc436559394)

[Understanding the algorithm: Poisson 35](#_Toc436559395)

[Implementing the 3 points (1D) and 5 points schemes (2D) 35](#_Toc436559396)

[A framework to handle the 2D schemes 35](#_Toc436559397)

[Performances: parallelisation 35](#_Toc436559398)

[Results 35](#_Toc436559399)

[Subjective remarks (logical and emotional) 36](#_Toc436559400)

[Summary and Conclusions 36](#_Toc436559401)

[Bibliography 36](#_Toc436559402)

[Annexe 40](#_Toc436559403)

[Annexe A: Splitting the Helmholtz Equation 40](#_Toc436559404)

[Annexe B.1: Taylor expansions 42](#_Toc436559405)

[Annexe B.2: One dimensional problem – Standard scheme 42](#_Toc436559406)

[Scheme of the interior point 42](#_Toc436559407)

[Scheme of the Sommerfeld boundary point 43](#_Toc436559408)

[Final schemes for all points 44](#_Toc436559409)

[Annexe B.3: One dimensional problem – Exact scheme 44](#_Toc436559410)

[Demonstration of the scheme 44](#_Toc436559411)

[Final schemes for all points 45](#_Toc436559412)

[Annexe B.4: Two dimensional problem – Standard Scheme 45](#_Toc436559413)

[Interior point 45](#_Toc436559414)

[Sommerfeld point 45](#_Toc436559415)

[Side points 46](#_Toc436559416)

[Corner points 46](#_Toc436559417)

[Class model of the framework 47](#_Toc436559418)

[Central Scheme Module 47](#_Toc436559419)

[Sommerfeld Scheme Module 47](#_Toc436559420)

[Simulation Module 47](#_Toc436559421)

[Reporting Module 47](#_Toc436559422)

[Table 1 - Classification of the linear 2nd order BVP 15](#_Toc436559423)

[Table 2 - Error using varied scheme of the derivative 24](#_Toc436559424)

[Table 3 - Computed p and C for each scheme ( 24](#_Toc436559425)

[Table 4. Two dimensional standard schemes 32](#_Toc436559426)

[Table 5. Two dimensional new schemes 33](#_Toc436559427)

[Table 6 -2nd, 4th, 6th order central point schemes coefficient 34](#_Toc436559428)

[Table 7 - 2nd and 6th order Sommerfeld schemes 35](#_Toc436559429)

[Table 8. One dimensional standard schemes 44](#_Toc436559430)

[Table 9. One dimensional exact schemes 45](#_Toc436559431)

[Figure 1: Detection and characterization of breast masses as a function of attenuation and speed of sound 10](#_Toc436559432)

[Figure 2 - Approximation of (taken from [***18***]) 21](#_Toc436559433)

[Figure 3 - Log (Err) vs. log (h) 25](#_Toc436559434)

*Extract of the instruction for the redaction of the final report:*

1. עמוד שער
2. תקציר
3. נושא הפרויקט: הצגת הבעיה והגדרת היעדים
4. רקע: בסעיף זה יוצגו ויוסברו מושגים היוניים להמשך
5. ניתוח הבעיה
6. מבנה הפתרון
7. תוצאות: סיכום מסודר של התוצאות (אם יש באלה – בתלות באופי הפרויקט, למשל גרפים, זמני ביצוע, בדיקות שנעשו וכדומה)
8. השוואת הפתרון המוצע הקיים היום והדגשת יתרונותיו
9. סיכום: מסקנות והצעות להמשך
10. ביבליוגרפיה
11. נספחים: הוראות להפעלת התכנה ונספחים נוספים לפי הצורך

הדו"ח יוגש למנחה באופן אלקטרוני בשני פורמטים (Word, PDF) או וצרוף zip של התכנה עם הנחיות הפעלה.

# Abstract

1. Numerous fields exhibit problems that motivate the study of ultrasound and tomography. An important set of medical problems is linked to ultrasound and tomography.
2. Solving one of these problems implies studying of the forward and the inverse problem of the wave propagation. There exist many mathematical model to the propagation of the wave and we chose one in particular
3. The treatment of this mathematical problem leads to one particular sub-problem: solving the Helmholtz equation: , with as a refractive index that depends on the space and the frequency, our model.
4. As many numerical methods maybe used to solve this problem efficiently we chose a particular one which is studied in more details here: the Finite Difference Method. The purpose of this method is to deduce efficient and compact schemes for a particular or model to be computed on a grid.
5. From learning the numerical method (by solving simpler model) and study our model (solve progressively complex variants of our model above) emerged the need for a more general tool. It would reduce the burden of the repetitive coding of simulation for different variant to its minimum. This allows to rapidly evaluating the correctness, efficiency of a variant, comparing them, impacting all the simulation when performance is improved.
6. Our task was to conceptualize such a tool and progressively integrate different feature to support wider range of hypothesis for the simulations as well as to search for a particular scheme that would solve our model.

# Presentation of the problem and definition of the objectives

Attenuation of ultrasound is very important, as it is a major factor in limiting the accessible depth for imaging. Attenuation is increased (and hence penetration of the beam reduced) for higher frequency (shorter wavelength) transducers. Standard (B-mode) ultrasound equipment intrinsically compensates for an expected average degree of attenuation by automatically increasing the gain (overall brightness or intensity of signals) for deeper areas in the anatomy.

Only a constant (average) value of the attenuation can be determined experimentally in B-mode ultrasound imaging. Measurements of the reflected signal alone (B-mode) do not contain enough information for determining the spatial dependency of attenuation in the anatomy. Tomography, namely taking into account scattering and transmission directions of the ultrasound waves, enables the measurement of attenuation. Ultrasound tomography is a promising new approach for breast imaging, for very recent reports see [[1](#LiC14)], [[2](#Hop14)]. However, methods for reconstructing attenuation images that are consistent with the observed frequency power law are presently lacking.

In this project I investigate methods of solving the Helmholtz equation corresponding to fractional wave equations. Such a Helmholtz equation is different than the standard one due to an explicit and non-trivial dependence of the refraction index on frequency. This frequency dependence accounts properly for the observed frequency power-law and is a result of using a fractional wave equation. The objective of using such Helmholtz equations, **which is the objective of this project**, is to provide the underlying support for consistent reconstruction of power-law attenuation and the corresponding speed of sound.

The tools built in this project enable a modular and flexible implementation of a variety of methods for solving the frequency-dependent attenuation in fractional Helmholtz wave equations, thereby achieving **another objective of the project**, namely the comparison of the performance and accuracy of several finite-difference methods of solution.

# Background

## Ultrasound: general characteristics

“By beaming high-frequency sound waves into the body, physicians can translate the "echoes" that bounce off body tissues and organs into "sound you can see," colorful, visual images that provide valuable medical information”[[1]](#footnote-2). The technique is very cheap (compared to other techniques such as CT (Computed Tomography), MRI (Magnetic Resonance Imaging), not harmful at all (fetal imaging), gives results in real-time (surgery) and is also extremely portable (moving ultrasound installation to the patient’s place is possible).

In standard (B-mode) ultrasound the image is created thanks to the information contained in the back-reflected waves (from the body organs). The acoustic stack is emitting and receiving only back-reflected sound waves. Images are constructed on the basis of the assumption of an average *speed of sound* and average *attenuation* that are independent of the location in the anatomy.

The following picture[[2]](#footnote-3) of Figure 1 shows detected masses for given sound speed and attenuation and a biopsy (sample of cells) revealed the nature of the detected mass. From this graph it is obvious that the above two parameters (speed of sound and attenuation) deserve to be measured in order to gain further important information, such as characterizing tissue and segregating malignant tumours from benign ones. As mentioned above, this information is simply not available with B-mode ultrasound devices, and that is the main motivation for using ultrasound tomography. In tomography the anatomy is surrounded with transducers, and waves that pass through it are measured, providing enough information for reconstructing speed of sound and attenuation.

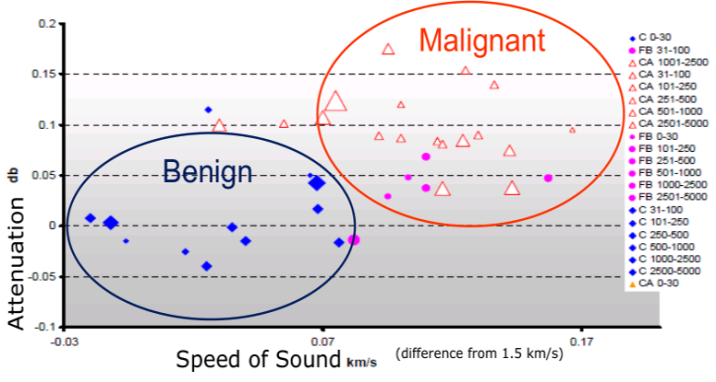


Figure 1: Detection and characterization of breast masses as a function of attenuation and speed of sound

Beside this, there is always the desire to increase resolution on the one hand and to access deeper organs on the other hand. The latter is limited due to attenuation. Indeed, better resolution may be obtained with high frequency, but attenuation also increases with higher frequencies and prevent the signal from reaching deeper in the tissue. In order to better understand this trade-off, a model is required that takes into account the speed of sound as a function of the location (2d or 3d) and the attenuation as a function of the location, as well as a function of the frequency.

## The physics of the problem

### Speed of sound and power law attenuation

The experiments show that attenuation follows a power low with an exponent in the interval of 0 to 2 that may be formulated in the following way [[3](#Duc90)]:

|  |  |  |
| --- | --- | --- |
|  |  | (1) |

Here is the location and frequency dependent attenuation, is the location dependent and frequency independent attenuation coefficient. The location is denoted by the space parameter and is the angular frequency related to the frequency () of the sound waves. is the location dependent exponent.

### Fractional wave equations from time to frequency domain

A possible model amongst many others [[4](#Cap67)], [[5](#Che04)], [[6](#Che03)], [[7](#Sza95)] that satisfies equation (1) is given by equation (2) below, proposed by [[8](#Kel08)] and [[9](#Kel081)]:

|  |  |  |
| --- | --- | --- |
|  |  | (2) |

Equation (2) is a Fractional Partial Differential Equation (FPDE) describing a power-law fractional wave equation.

Note that for , equation (2) reduces to the usual wave equation

|  |  |  |
| --- | --- | --- |
|  |  | (3) |

The approach adopted here is to take the temporal Fourier transform of the pressure wave define as:

|  |  |  |
| --- | --- | --- |
|  |  | (4) |

This allows us to rewrite (2) as:

|  |  |  |
| --- | --- | --- |
|  |  | (5) |

Note that for equation (5) reduces to the usual Helmholtz equation

|  |  |  |
| --- | --- | --- |
|  |  | (6) |

Define a refractive index by (7) below,

|  |  |  |
| --- | --- | --- |
|  |  | (7) |

making it possible to rewrite equation (5) as:

|  |  |  |
| --- | --- | --- |
|  |  | (8) |

## Frequency-dependent attenuation in the Helmholtz equations

Equation is no more than the Helmholtz equation already well known in the literature, but with a slight change that adds an additional degree of complexity: the refractive index is a function of space and the frequency. Methods for solving the frequency independent refractive index case are well studied in the literature. However, there is a need to further understand the role of the frequency dependent refractive index of equation (7) in the solution of equation (8).

At high frequencies, the numerical solution of equation (8) is very difficult, due to the oscillatory nature of the resulting pressure wave . By considering a solution of the form

|  |  |  |
| --- | --- | --- |
|  |  | (9) |

where is the amplitude and is the travel-time, one obtains the following two coupled equations (see )

|  |  |  |
| --- | --- | --- |
|  |  | (10) |

|  |  |  |
| --- | --- | --- |
|  |  | (11) |

Equations (10) and (11) are [two-way] coupled. In cases where and are relatively non-oscillatory, there is an advantage in solving them instead of solving equation (8) directly. Furthermore, in the high-frequency limit, the middle term of equation (10) can be neglected, and one obtains a frequency-dependent Eikonal Equation that is independent of the amplitude

|  |  |  |
| --- | --- | --- |
|  |  | (12) |

Equations (11) and (12) are [one-way] coupled, i.e. the gradient solved for in the Eikonal equation (12) should be inserted in the transport equation (11) for the amplitude .

## *Boundary values*

In order to solve any PDE (Partial Differential Equation) such as the ones encountered above or even any ODE (Ordinary Differential Equation) one must fix the Boundary Conditions. Indeed, such equations have infinite solutions and only the boundary conditions may transform the problem from an ill-posed to a well-posed [[10](#Run)] one. The equation together with its boundary conditions is called a Boundary Value Problem.

There are various ways of applying constraints at boundaries and they express the nature of the corresponding physical system.

In the case of an interior problem [[10](#Run)] with solution **,** the system is considered in a limited area, the bounded domain () and the condition at the boundary () may be expressed by:

* ,whenthesolution is directly specified at the boundaries
* , when the derivative is specified at the boundaries
* , Cauchy when both are known
* , Robin when a linear combination of both the solution and the derivative are known.

The list is not exhaustive [[11](#Goc02)] but the above are the main ones.

In the exterior problem [[10](#Run)], the region of the solution is unbounded. Physically, an incoming wave is entering the simulated region, possibly interfering with artefacts and continues its way towards the infinity without any back reflecting waves returning to it. The source may be modelled by Dirichlet condition as we know its value. However, modelling the propagation requires absorbing condition:

* , the Sommerfeld condition in the particular case of the Helmholtz equation,
* , Damping technique where we avoid reflection by simulating and absorbing layer. This is equivalent to Sommerfeld.

Note that these solutions at the boundaries are effective solutions i.e. it is possible to substitute them in the equation and check that it is verified.

# Analysis of the problem

## General considerations

* The range of frequencies requires the adaptation of two different treatment approaches, namely, the ray model for high frequencies, and the solution of the full Helmholtz equation for the low to middle frequency range.
  + The former requires dealing with the Transport and the Eikonal equations. The Transport equation is a first order and linear partial differential equation, resulting in rather straightforward methods, while the first order non-linear Eikonal equation can be treated with finite-difference methods, such as the Fast Marching Method (FMM) [[12](#Set99)];
  + For the second more difficult numerical case (second order linear partial differential equation), the selection of differential equation numerical solver is important.
* We must not forget to include specific boundary conditions in all the above equations.
* The implementation require a tool chain from a possible computation package to the different output that we need to set up and may require some development.

## Choice of the Helmholtz equation

As mentioned, there are two main ways to treat the problem of solving equation (8): solving the Helmholtz equation directly or computing the Eikonal equation and using its output as an input to the Transport equation. The latter is possible after simplifying equation (10) with the approximation of high frequency. For low frequency, it is possible to solve the Helmholtz equation (as equation (10)and (11) are just a reformulation). However, it is still not clear until what range of frequencies it is possible to compute a sufficiently precise solution before the oscillatory behaviour begins damaging the precision of the simulation. This point of view is of great interest as it does not require supplementary simplifying hypothesis.

The Helmholtz equation problem is thriving in the research community as: it plays a central role in numerous fields of the research; it involves a variety of formulations (time dependent, time independent) with appropriate boundary conditions; it models specific geometry parameters of the region and other constraints, such as refraction index (in our case), as well as the non-homogeneous formulation. It is also studied as a prototype to demonstrate progress in the field of computation (study of memory consumption and parallelisation [[13](#Heg10)], specific algorithm, execution time vs. precision [[14](#Eli12)]). It was necessary to extract, out of the wealth of published material, the relevant techniques that are useful to solve our particular problem.

## Choice of the numerical method

Although it is sometimes possible to arrive at closed form solutions to PDE, such as the Helmholtz equation in our particular case, one has no other choice but to use numerical methods when the problem becomes complex.

Second order PDEs are generally classified according to their determinant [[15](#Kum11)]. For a general linear PDE:

The determinant is expressed by: and we have:

|  |  |  |
| --- | --- | --- |
| Value of | Classification | Example |
|  | elliptic |  |
|  | Parabolic |  |
|  | hyperbolic |  |

Table 1 - Classification of the linear 2nd order BVP

This classification corresponds respectively to: equilibrium, propagation and eigenvalue problem [[15](#Kum11)]. Depending on the type of problem and very often the physics of the problem simulated, some specific techniques have been developed. In the following, we introduce the reader with the major methods used to compute solutions of PDE. These methods are very general and give birth to a wide range of numerical techniques. I have studied in-depth the following four alternatives: the Finite differences, Finite elements, Finite Volumes and the Spectral Methods. The last three are presented in Appendix …

### Finite differences

This is the numerical method that has been chosen for studying and model the Helmholtz equation in this project. The reader will find more details in the analysis presented in this report.

The method belongs to the mathematical field of analysis theorems, tools and methods. In brief, in this method we describe the region of our Boundary Problem on a *grid* (not necessarily uniform) of spacing (). During the simulation the solution () is computed at each point with the help of a formula (or *scheme*). The scheme is obtained by *approximating* the PDE by finite difference i.e. a formula that gives as a function of its neighbours (not necessarily its immediate neighbours). The method is associated with a structural *truncation error*.

As straightforward as the idea may be the following challenges are faced while formulating the scheme and implementing the method:

* How can we seek the maximum degree of precision (high order of the truncation error) for a minimal number of neighbouring points involved?
* How to handle [and how to translate to schemes] the various boundary conditions?
* Is the scheme sufficiently flexible to welcome some changes? For example, if the original problem is changing to a non-uniform formulation, i.e. a constant becomes a function of the variable of the problem (as in our refractive index)?
* How about the trade-off: high resolution grid vs. computational complexity and long running times?
* How about geometrical changes over the domain?

Introductory material: [[16](#Cha10)] [[17](#Bur10)]

For an in-depth and more exhaustive cover of the method: [[18](#LeV07)] [[19](#JWT95)] [[20](#Str89)]

### Finite elements

This method is a bit more elaborated. It originates in engineering where some modelling is necessary to represent different constraint applied to composite material with variable geometry. This is only after that it was used to solve PDE numerically.

The domain over it we want to model the phenomena is divided in joined *element* at point called *nodes* forming a *structure* arrange in a *mesh*. Each element is awarded with a small simple function generally a polynomial and the whole solution is approximated element by element over the whole structure.

Some simple (one dimensional linear structure) and average (2D involving well studied geometric element) time independent problems in physics may be solved from here by so called direct methods: generate a matrix corresponding to the physics and geometry of the element, provide loads to nodes, boundary conditions and solve the system of algebraic equations.

When modelling PDEs this approach is insufficient. There are two main methods: the Rayleigh-Ritz method (or Variational Method) and the Galerkin method (and its variations). Both involve moving the problem from a *strong form* (the original PDE) to a *weak form* (most of the case the integral of the problem) or *variational form* called a *functional* that contains the original equation in its integral representation. Both forms are equivalent but the strong form requires that the conditions of the BVP may be respected at all point whereas the weak form allows them to be so in average over the integral. However: “[…] for some applications the functional needed for a variational approach cannot be written.[…] FE (Finite Element) for such problems can still be obtained using weighted residual methods of which the Galerkin method is the most widely used” ( [[21](#Coo02)], p.194 ). In the Galerkin method the functional take the form of a *residual* (also a function) to which a *weighted function* is introduced before taking the integral. There exist many other weighted residual methods.

The advantage ( [[21](#Coo02)] ):

1. The method is applicable to virtually any physical field,
2. Versatility of the geometry of the mesh (flexible geometry), higher precision may be obtained by increasing the resolution around some specific points,
3. Different physical, mathematical properties and constraints may be combined at each nodes of the mesh,
4. The integral form allows a certain robustness of the method at singularities or problematic points.

Introductory material: [[16](#Cha10)] [[17](#Bur10)] [[22](#Sch06)]

For an in-depth and more exhaustive cover of the method: [[21](#Coo02)], [[23](#The13)], [[24](#Goc06)](All methods), [[25](#Joh88)], [[26](#Axe01)], [[27](#PSo06)] (treatment of PDE).

### Finite Volumes

It is very similar in its philosophy to the finite element method.

The particularities are that the region is divided to finite volumes cells. The PDE problem is also transform to an integral form that is built as an application of a Conservative Law. At each cell level and over the whole region we require this constraint to be respected.

The use of a Conservative Law make the problem suitable to the establishment of a model of fluid dynamics where we can require for instance that the algebraic some of the input and output over a volume may be constant. This technique is widely used to solve hyperbolic BVP such as fluid dynamics equations, the Wave equation or Advection and Diffusion equations therefore the literature is often directed to this kind of problems.

Introductory material: [[28](#JPe05)], [[22](#Sch06)]

Treatment of hyperbolic PDE: [[29](#Lev04)]

### Spectral Methods

The Spectral Method introduces a novel view to the problem and reuses some techniques of the preceding methods.

As the solution of a BVP may be approximate by a function, this one has a representation in different basis: Fourier basis for periodic problems and Chebyshev or Legendre polynomial for non-periodic problems. The solution is expressed in terms of this new basis (namely a finite sum) and the best approximation is sought for the coefficient in this basis. There are roughly three main methods:

1. The *Galerkin method (a Weighted Residual Method)*: the problem is converted to its weak form involving the integral of the *residual function* for which the coefficient in the new basis are the unknown.
2. The *Tau Method* (or pseudo spectral method): the coefficients are solution of the finite sum at the boundaries of the integral in the weak form.
3. The *Collocation Method*: the finite sum is required to be satisfied over the nodes of a non-regular grid similarly to the finite difference.

The first and third methods give birth to an algebraic system of equations.

There are some interesting properties that stem from this new representation for the solution such as better precision.

Sources: [[30](#AKo09)], [[31](#Tre96)], [[32](#Boy00)], [[33](#Tre01)]

### Discussion

Our problem is to find the solution to Helmholtz equation:. Our version differ from the classic one in that is a function of a space vector () and of the frequency (). We are also interested in better understanding of the limit at which the oscillation caused by increasing frequency becomes disruptive for the precision of the simulation. This equation withhigh frequency and higher dimensions remains a challenge to the research community. Therefore it seems rational to start with the simplest method, namely the Finite Differences method.

As noticed in the Appendix, the Finite Elements method seems very promising also. It was historically created to deal with irregular geometry of the region as well as with changing properties of the material and physical constraints. It requires converting the problem to a weak form (variational for the Rayleigh-Ritz method or residual for a weighted residual method such as Galerkin method), generating the mesh for the region and choosing/comparing some simple polynomial function for the element which require some mathematical refinement. It is interesting to realize that the Finite Difference method may be thought of as a particular case of the Finite Element Method ( [[34](#OCZ06)] ). This led us to consider the more general Finite Elements method to be more complex to implement as compared to the Finite Differences one.

As discussed in the Appendix, the Finite Volumes method has been developed to answer problems that may be expressed with conservation law which doesn't quite fit our problem. Nevertheless, there is some interesting work done on electromagnetic field problems using Maxwell equations in which the law of conservation of energy is used for the weak form [[35](#Har10)], [[36](#EHA01)].

The Spectral Methods (Galerkin or weighted residual version) is also quite promising. This approximation is estimated over all domain points, instead of the direct or close neighbours as in the Finite Difference method, making use of multiple overlapping polynomials over the domain, instead of a polynomial function per element as in the Finite Elements method ( [[32](#Boy00)], Introduction ). However it is a challenging method as it requires advanced tools of mathematics when trying to master the method. There is some interesting work that has been done on the Helmholtz equation with a constant ( [[37](#She05)] ) with absorbing conditions in a circular domain, but nothing has been attempted for variable and high wave numbers.

The above led us to adopt the Finite Differences method as the method of choice for studying the Helmholtz equation in our case.

## The finite difference method (FDM)

### Introduction

We will now present the main aspect of the FDM that more particularly allow to understand our problem but first of all we recall to the reader the goal of the method.

The intent of a finite difference equation or *scheme* is to provide and approximation of the solution of the whole BVP at a particular *point* of the grid possibly taking into account boundary condition. In order to solve a particular BVP over the whole considered *domain* we seek a set of such equations for central, side and corner points.

In the first section, the main mathematical equations that allow deriving the most common schemes are presented with some basic techniques to derive them from the Taylor expansion. Following this a short example will give an explanation about the truncation error that is structural to a given scheme when using this method, particularly the effect of widening the number of neighbour’s points on the order of the error. In the third part, the reader will be introduced with a first example concrete namely the Laplace equation that although not treating directly with the Helmholtz equation cumulate the advantages of being: a simple case of an *elliptic problem* (with a shared operator with the Helmholtz equation) and a two dimension problem and reveal the treatment of the fundamental Dirichlet boundary condition. Eventually, we will walk through the different type of schemes for the Helmholtz equation that have been studied from half a dozen publications:

1. A classical scheme gives a solution for constant with the most common available scheme. It allows checking that the method is understood and that the absorbing boundary condition may be integrated to it [[13](#Heg10)]. It also serves as a reference for the other methods.
2. The Exact Scheme that naturally sounds very attractive as it claims to give an approximation nearly equal to the closed-form solution [[38](#YAU01)], [[39](#TZh12)], [[40](#Lam03)]. It covers the 1D and 2D case with constant only.
3. A couple of compact schemes of 4th and 6th order that support variable (dependence on the space variable) and non-homogeneous formulation (, with a function of space and time) [[14](#Eli12)], [[41](#Erl12)], [[42](#Isa94)].

For the first three section I have learned from: [[17](#Bur10)], [[16](#Cha10)], [[20](#Str89)], [[18](#LeV07)].

### Basic Scheme for order 1 and 2 operators

This section presents the fundamental ideas behind the construction of schemes i.e. the derivative and Taylor expansion.

#### Derivatives

Suppose that we want to approximate the derivative of a function at some point from its immediate neighbours. The first idea, and the more natural, is to go back to the definition of the derivative. The following figure state the first possibilities:

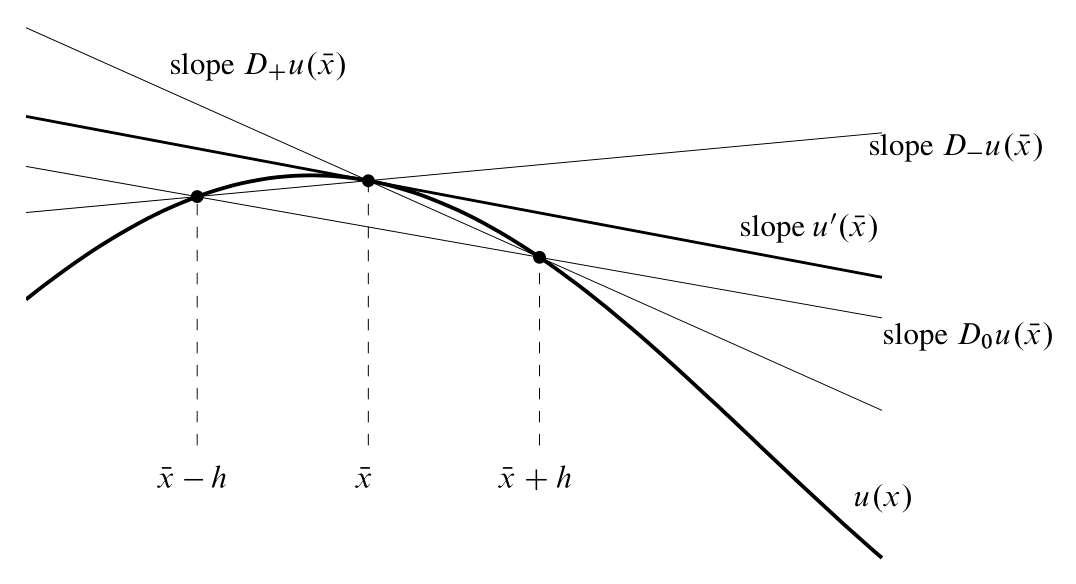


Figure 2 - Approximation of (taken from [[18](#LeV07)])

In Figure 2 - Approximation of (taken from [[18](" \l "LeV07)])Figure 2 we show that we may include in our computation the point of interest with either the following point or the preceding point or even attempt to make an average of both values. The definition of the limit gives: from which we could derive the following approximations:

|  |  |  |
| --- | --- | --- |
|  |  | (13) |

|  |  |  |
| --- | --- | --- |
|  |  | (14) |

|  |  |  |
| --- | --- | --- |
|  |  | (15) |

As we get rid of the original limit it is important to note that (13), (14), (15) are just approximation and it tend to be closer to the search derivative when become smaller.

However, there are two problems with this formulation. It is not so easy to find how to express higher order derivative say order two derivative and we need such derivative to continue building the scheme for our equation. What is our expectation concerning the precision of these schemes or what about their *order of accuracy*? This is realized with the Taylor theorem.

#### Taylor Expansion

The Taylor expansion state that at the neighbourhood of a point for an infinitely differentiable function:

|  |  |  |
| --- | --- | --- |
|  |  | (16) |

With the change of variable , this may be rewritten:

|  |  |  |
| --- | --- | --- |
|  |  | (17) |

Note that we include the numerous terms of higher order value under the notation with its usual mathematical meaning[[3]](#footnote-4). We may re-write this expansion for other neighbouring points:

|  |  |  |
| --- | --- | --- |
|  |  | (18) |

|  |  |  |
| --- | --- | --- |
|  |  | (19) |

|  |  |  |
| --- | --- | --- |
|  |  | (20) |

This formulation is very powerful as it allows us to have an idea about the order of accuracy of the remainder of our approximation. The truncation error is now a polynomial of known order. Also we may form other approximation much less intuitive that the ones we saw in the preceding section by including farer neighbouring points in our equation of the scheme.

It is easy to see that (13) is obtained by (17), (14) is obtained by (18) and (15) is obtained by both (17) and (18). The truncation error is in for the two first schemes and for the last scheme.

However it is possible to reach more precise scheme if we include other points. For instance combining (17), (18), (20) gives the following scheme:

|  |  |  |
| --- | --- | --- |
|  |  | (21) |

We will use this scheme in the next section that deals more deeply with errors.

Eventually, the Taylor expansion allow to form schemes for higher order such as order 2 that we also will need in our schemes of the Helmholtz equation.

Thus, from equation (17) and (18) we may obtain:

|  |  |  |
| --- | --- | --- |
|  |  | (22) |

Note that all these schemes have been given for a one dimension function but they may be combined in order to form some higher dimension scheme 2D or 3D for instance.

### Truncation Error

In this section a better understanding of the error is pursued through an example and a brief discussion. In practice we want to check that the scheme behaves as expected given a set of parameter for a simulation. It basically tests the implementation but also as the frequency goes up, we expect some decays to occur and this may help to identify the breakaway point.

#### Sin(x) example

In this simple example, reproduced from [[18](#LeV07)], the general schemes: (13), (14), (15), (21) are used to approximate the value of the derivative of the function (i.e.) around the point 1 with different values of step . From this value the error is computed with the analytic solution namely . The point is that from the Taylor expansion and for an error of order of accuracy we expect some error of the form: . It means that: or equivalently:

|  |  |  |
| --- | --- | --- |
|  |  | (23) |

The procedure that produces both the following table and the graph has been written completely as an exercise and is part of the delivered code. Results are sum up hereunder:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *'h'* | *'Back Err'* | *'Forw Err'* | *'Cent Err'* | *'du\_3\_err'* |
| 1.0000E-01 | -4.1138E-02 | 4.2939E-02 | 9.0005E-04 | -6.8207E-05 |
| 5.0000E-02 | -2.0807E-02 | 2.1257E-02 | 2.2510E-04 | -8.6491E-06 |
| 1.0000E-02 | -4.1983E-03 | 4.2163E-03 | 9.0050E-06 | -6.9941E-08 |
| 5.0000E-03 | -2.1014E-03 | 2.1059E-03 | 2.2513E-06 | -8.7540E-09 |
| 1.0000E-03 | -4.2065E-04 | 4.2083E-04 | 9.0050E-08 | -6.9979E-11 |

Table 2 - Error using varied scheme of the derivative

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | 'fitting' |  |  |
| 'p' | 1.0041578 | 0.995453297 | 1.999908359 | 2.994740169 |
| 'C' | 0.431483649 | 0.409330432 | 0.09000255 | 0.067869913 |

Table 3 - Computed p and C for each scheme (

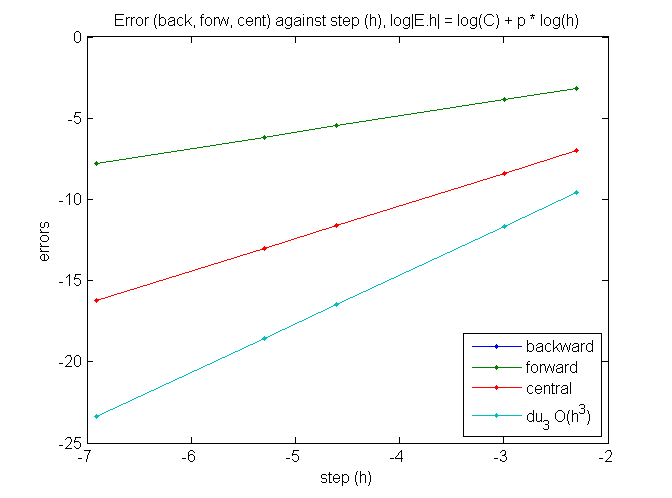


Figure 3 - Log (Err) vs. log (h)

#### Discussion

Firstly Figure 3 confirm the linear relationship we have in (23) and the steeper slope from the top lines to the bottom one shows and increase in the order of the polynomial. The following discussion explains the reason of it.

Table 2 shows a similar order of error in the first two columns. That is expected as we took basically the same scheme formula (backward point vs. forward point). In Table 3 the preceding result are correlated to the result first two columns. So the order of the error is a polynomial in with . This result is also expected as from (17) we can derive:

|  |  |  |
| --- | --- | --- |
|  |  | (24) |

This gives us the basic formula of the derivative or (13) (once neglecting the remainder) added up to a polynomial of higher order (in bold) but with a main term in . The same basic reasoning applies to the scheme with the backward point.

The central point is derived from the combination of (17) - (18) that allows us to get rid of the second derivative and leaves us with two times the first derivative and a polynomial of order 2:

|  |  |  |
| --- | --- | --- |
|  |  | (25) |

So this time the remainder is in wich is also computationally verified from the value of in the third column in the third column of Table 3.

It is possible to appreciate here the power of the Taylor derivation when it comes to include some more distant neighbouring point and build an ad-hoc scheme of desired precision such as the scheme (21) that order of accuracy is 3.

There is an automatic method to deduce coefficient when expressing a derivative as a function of its neighbouring points. However, in practice the use may be limited as experimental data may not furnish enough points around the simulated domain and one may often content itself with lower, less accurate but compacter order scheme.

The breakthroughs operated by the last scheme that we have analysed for the Helmholtz equation (see the last section of this part) challenges this disturbing fact as it propose increasing the order of accuracy of the scheme by using just the set of immediate neighbours however enlarged to the diagonal points. This is done in return of an increasing complexity.

### A first practical case: The Poisson Equation

Now that the tools are gathered in order to build basic operators and that some practical insights have been given about the truncation error evaluation inherent to the method a first practical case may be introduced that concretely put the method in use.

The Poisson is very classical when introducing the functioning of the FDM on a non-trivial 2D elliptic BVP [[16](#Cha10)], [[17](#Bur10)], [[18](#LeV07)]. The reasons it is also presented here despite not directly dealing with the Helmholtz equation is multiple. First it was a concrete part of the learning process of acquiring the FDM technique to reproduce some cases from the preceding cited works. Secondly, the Poisson problem is very similar to the Helmholtz equation as it is an *elliptic case* corresponding to a steady state (or equilibrium) often studied in *two dimension* which is our constraint for the Helmholtz BVP. Eventually it gives an example of analysis for a non-regular grid that is more general that the regular one. Solely the Dirichlet boundary condition but not the Sommerfeld one is put in practice which only partly covers our needs.

We warn the reader that only the process taking place between stating the physical problem until its expression in term of FD schemes is redrawn here. The presentation of the algorithm and its implementations is postponed to Architecture of the algorithm and code. The reason is that, from their analysis, conclusion were gradually drawn that led to a second followed by a third and final implementation under the desire of progressively include additional schemes. With this condition it felt more logic to start the argumentation from this point.

#### BVP

##### Physical context

The purpose is to solve the Elliptic Poisson Partial Differential Equation with help of the FDM. More particularly we solve it with a five point difference scheme in two dimensional space and Dirichlet Boundary Condition. The explanation about the method has been taken from [[17](#Bur10)] and [[16](#Cha10)].

The problem comes historically from the following Heat Equation of Fourier:

|  |  |  |
| --- | --- | --- |
|  |  | (26) |

In two dimensional spaces and for any general real function in may be written as below:

|  |  |  |
| --- | --- | --- |
|  |  | (27) |

We note that the function is not anymore dependent of time. For instance, concerning the Heat Equation, it corresponds to the steady-state regime. In the particular case of, the homogeneous version of equation (27) is known as the Laplace Equation.

##### Discretization

The problem is discretized over a rectangular area with the abscissa: and. The step over the abscissa is given by and over ordinates by. The coordinate of any point in the grid is therefore given by:

|  |  |  |
| --- | --- | --- |
|  |  | (28) |

The Taylor series on let us generate the symmetrical difference formula for the second order partial derivation of.

|  |  |  |
| --- | --- | --- |
|  |  | (29) |

And the Poisson Equation may be written as:

|  |  |  |
| --- | --- | --- |
|  |  | (30) |

##### 5-points Finite Difference Scheme

By considering the higher order terms as negligible and by multiplying each side by, the equation (30) lead to the following general scheme in the case of an irregular step-size grid:

|  |  |  |
| --- | --- | --- |
|  |  | (31) |

In the particular case of a regular grid of identical step size () along the abscissa and the ordinates one obtains the now widespread formula:

|  |  |  |
| --- | --- | --- |
|  |  | (32) |

#### Discussion

The set of equations given in (32) describes the way to compute the value of at each point. The value of over the whole domain is given by the reorganised vector solution of an algebraic system that is formed by computing what occurs at each point.

We see that the scheme equations are very dependent of the choice of the grid or more generally of the geometry of the domain. This is a characteristic of the method that we raised in Finite differences that is obvious when at the moment we define the grid. The analysis process must be done once again if the domain is for let say a circle.

Another interesting fact is that in the case of a homogeneous equation the central scheme (the first equation in (32)) is completely independent of the step taken. Its sole influence come from the application of the boundary condition such as Dirichlet where a concrete value of the function must be computed (or taken from experimental data) in order to the local boundary equation.

### Schemes for the Helmholtz Equation

A definition of the boundary value problem for the Helmholtz equation will be given in the next section followed by the main schemes that have been studied.

During the project the first two schemes have been studied together. The first although was not expected to give good practical result was thoroughly studied essentially for its pedagogical value and as a reference for comparison. It was also motivated by reproducing the result presented in [[38](#YAU01)], our main source to study and implement the Exact Scheme that permanently gave comparing result with the Classical one however (almost) not giving any explicit indication on its writing or for its implementation and particularly the delicate matter of the Sommerfeld boundary condition. So we had to learn from [[13](#Heg10)] and re-build by demonstration a set of schemes that could allow computing the same closed solution that is exhibited in [[38](#YAU01)].

After some struggling, the Exact Scheme has been abandoned for reasons that will be given in the part treating of the result. We then turn our interest to another implementation that although not pretending to “exactness” was attractive at many views: a very respectable order of accuracy, some integration for non-constant (we remind that in , generally a constant) and the possibility to compute inhomogeneous cases also .

During the first part of the project (study of the first two schemes), the one-dimensional cases have been also studied (and solved) both for their pedagogical value and to compare them with the results of the original article. However it required some work we chose to put their relative information in the annexe as it could diverts and tire the reader while not bringing new concepts to the two dimensional case treated hereunder. See Annexe B1, B.2 and B.3 for more detailed analysis of the one-dimensional cases schemes.

#### Presentation of the boundary value problem

The Boundary Value problem of the Helmholtz equation takes the following form:

|  |  |  |
| --- | --- | --- |
|  |  | (33) |

Here (: the celerity of the wave, : the period, : the frequency, : the wave length).

The solution is a function of a two component vector (two dimensional case) over a given domain. The discretization of the latter must not be particularly on the basis of a regular grid but all the studied schemes adopted this hypothesis as it greatly simplifies the schemes equations (compare for instance (31) to (32)) together with the implementation.

The Sommerfeld boundary condition take the theoretical form of a limit [[43](#Moo88)] but it generally has this more usable form in most of the article and being a normal vector to the domain. might vary depending on the closed solution problem used to illustrate the scheme but generally with . We remind that if solving the Helmholtz equation as exterior problem, the Sommerfeld boundary condition express the fact that the wave propagates toward the infinity without coming back waves. The BVP is well posed if this condition is *not* applied on the boundary of the whole domain. Physically we need a source and that is why Dirichlet boundary condition also appears in the BVP.

#### Classical scheme (2nd order)

## The two dimensional problem

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

|  |  |  |
| --- | --- | --- |
|  |  | (34) |

The following schemes may be calculated from the second order Taylor series. The vector 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. Sommerfeld boundary conditions may not be applied to the whole boundaries.

### 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 between the Sommerfeld constraint applied on the corner points (NE, SE, SW, NW). Because of the nature of the derivation (along the normal vector (43)) in the Sommerfeld condition, the results is not directly obtained from the definition and is demonstrated later see Annexe B.4: Two dimensional problem – Standard Scheme.

|  |  |
| --- | --- |
| Points type | Scheme |
| Interior |  |
| Dirichlet |  |
| Sommerfeld (east boundary) |  |
| Sommerfeld (west boundary) |  |
| Sommerfeld (north boundary) |  |
| Sommerfeld (south boundary) |  |
| Sommerfeld (north-east corner boundary) |  |
| Sommerfeld (south-east corner boundary) |  |
| Sommerfeld (south-west corner boundary) |  |
| Sommerfeld (north-west corner boundary) |  |

Table 4. Two dimensional standard schemes

### Exact Scheme

For a demonstration of the following scheme see [[40](#Lam03)] and [[38](#YAU01)].

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

|  |  |
| --- | --- |
|  | (35) |

The general schemes that are given by [[38](#YAU01)] are recalled here:

|  |  |
| --- | --- |
|  | (36) |

The parameter is the Bessel function defined by: and is currently available on most mathematical computational platform. The parameter 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 directly deduced from (36).

|  |  |
| --- | --- |
| Points type | Scheme |
| Interior |  |
| Dirichlet |  |
| Sommerfeld (east boundary) |  |
| Sommerfeld (west boundary) |  |
| Sommerfeld (north boundary) |  |
| Sommerfeld (south boundary) |  |
| Sommerfeld (north-east corner boundary) |  |
| Sommerfeld (south-east corner boundary) |  |
| Sommerfeld (south-west corner boundary) |  |
| Sommerfeld (north-west corner boundary) |  |

Table 5. Two dimensional new schemes

### Compact 4th and 6th order schemes

This section presents a set of schemes resulting of the work involving some common people see [[44](#Bay83)], [[42](#Isa94)], [[45](#Sin04)], [[46](#Sin06)], [[41](#Erl12)], [[14](#Eli12)], [[47](#Dan12)] that revolve around the same ideas in the way it treats the Helmholtz equation namely taking a larger set of point into account.

The main advantages of these schemes are: order of accuracy, compactness, working for inhomogeneous cases and recently integrating some possibilities for variable.

##### Formalisation of the problem

We may state the problem as: with being the solution and the index and a known function. We are voluntarily informal concerning the element of the equation as depending on the scheme they may be allowed to be function in certain cases. If it exists a (compact) scheme involving all the neighbouring points of an approximation, it will be written as:

With:

And:

In the same fashion, for:

And:

With a set of coefficient that explicitly need to be found:

This formalism, however simple and not giving a direct solution to our problem, is still powerful at many views. Firstly it is limited to a 9 points expression but may be used to express any operator (meaning any other PDE such as Poisson and we will). Secondly it groups the points so that it is easy to visualize the coefficient common to the points and the complexity added by higher order schemes. Eventually, it helped greatly in the design of the framework that we detail in the following part (see Architecture of the algorithm and code).

##### Schemes

The set of scheme given here concern the homogeneous form of the equation (meaning).

|  |  |  |  |
| --- | --- | --- | --- |
| *Order* |  |  |  |
| **2nd** |  |  |  |
| **4th** |  |  |  |
| **6th** |  |  |  |

Table 6 -2nd, 4th, 6th order central point schemes coefficient

There is some concrete indication of the value of and in [[41](#Erl12)] and [[47](#Dan12)] for instance.

Similarly to above and in order to apply the Sommerfeld boundary condition we introduce the formalisation for a general Sommerfeld scheme that:

The index is unique as this equation characterise what is happening at a border only. The indices stand for *before* (interior point), stands for forward or after (exterior point) and just as in the preceding formulas stand for the central or “on the boundary” point. We have the following table for a 2nd and 6th order schemes:

|  |  |  |  |
| --- | --- | --- | --- |
| *Order* |  |  |  |
| **2nd** |  |  |  |
| **6th** | ) |  |  |

Table 7 - 2nd and 6th order Sommerfeld schemes

In Table 7, has the same meaning as explained in Presentation of the boundary value problem.

# Architecture of the algorithm and code

## Choice of the technologies

## Understanding the algorithm: Poisson

## Implementing the 3 points (1D) and 5 points schemes (2D)

## A framework to handle the 2D schemes

## Performances: parallelisation

# Results

Numbers and graphs accompanied by description, comparisons, surprises etc.

Discussion – highlights of the above, i.e. the two main results

# Subjective remarks (logical and emotional)

Some transversal consideration had to be taken into account. The mathematics of numerical analysis that deal with solving differential equation are quite complex, and are generally introduced at the end of a course in numerical analysis. On one side we could not afford for this type of project giving to much weight to the theoretical background before starting to try some practical methods. On the second, mind must be kept sufficiently open as the project could evolve as soon as some directions gave profitable results.

# Summary and Conclusions

What was achieved (use all the titles above for this description)

What was planned vs. what was done (supported by Gantt)

Future recommended work

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x

# Annexe

## Annexe A: Splitting the Helmholtz Equation

We wish to explain how the two equations (10) and (11) are obtains from equation (8) by plugging equation (9). This will be shown for the three dimensional space, but other dimensionalities are easily understood from it.

Let be a function of a vector sufficiently smooth (at least two times derivable):

The gradient operator in three dimensions is defined as:

Applied to our function it gives:

|  |  |  |
| --- | --- | --- |
|  |  | (37) |

|  |  |  |
| --- | --- | --- |
|  |  | (38) |

Let be the ansatz solution given in equation (9):

We will develop the second derivative term of equation (8):

Calculation in one dimension for:

Similarly for and :

Summing up the three equations one gets

Rearranging terms

By inspecting equations (37) and (38) one gets

Now the generalized Helmholtz equation is

|  |  |  |
| --- | --- | --- |
|  |  | (39) |

By defining

One arrives at

|  |  |  |
| --- | --- | --- |
|  |  | (40) |

By requiring separately that the real part and the imaginary part in equation (50) are equal to zero, one arrives at equations (10) and (11).

The two dimensional case is trivially done in the same way, just omitting the z terms.

## Annexe B.1: Taylor expansions

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

|  |  |
| --- | --- |
|  | (41) |

|  |  |
| --- | --- |
|  | (42) |

## Annexe B.2: One dimensional problem – Standard scheme

The BVP is expressed as:

|  |  |  |
| --- | --- | --- |
|  |  | (43) |

### Scheme of the interior point

By adding (41) and (42) we obtain the central difference:

And from equation (43) we may build the scheme:

That gives directly the interior point scheme:

|  |  |
| --- | --- |
|  | (44) |

### Scheme of the Sommerfeld boundary point

By subtracting (42) from (41) we obtain the following approximation that is called the central scheme for the first order derivative:

|  |  |
| --- | --- |
|  | (45) |

And the Sommerfeld constraint of (43) may therefore be written as:

And this lead directly to the following scheme:

|  |  |
| --- | --- |
|  | (46) |

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 from equation (46) in the central difference point (44). Alternatively, an expression of may be built from (46) and replace in equation (44) and this for the leftmost point. This lead directly to the scheme expression for Sommerfeld written in: **Table 8**.

For instance, the left extremity may be described this way:

That gives:

### Final schemes for all points

This is a sum up of the scheme for all possible point that were used for a concrete implementation.

|  |  |
| --- | --- |
| Points type | Scheme |
| Interior |  |
| Dirichlet[[4]](#footnote-5) |  |
| Sommerfeld (right) |  |
| Sommerfeld (left) |  |

Table 8. One dimensional standard schemes

## Annexe B.3: One dimensional problem – Exact scheme

The general schemes that are given by [[38](#YAU01)] 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.

|  |  |
| --- | --- |
|  | (47) |

### Demonstration of the scheme

The full demonstration of the formulas that are used to build the schemes may be found in [[40](#Lam03)] [[38](#YAU01)] and [[39](#TZh12)].

### Final schemes for all points

|  |  |
| --- | --- |
| Points type | Scheme |
| Interior |  |
| Dirichlet |  |
| Sommerfeld (right) |  |
| Sommerfeld (left) |  |

Table 9. One dimensional exact schemes

## Annexe B.4: 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 (41) and (42) in their two dimensional version:

This gives us and expression for the second order derivative and we deduce the following central point scheme from equation (33):

And by multiplying each side by we find the expression of Table 4.

|  |  |
| --- | --- |
|  | (48) |

### Sommerfeld point

We recall that from equation (33) we have the following Sommerfeld condition: with 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 axis for the east and west side of the region and the unit vector along the 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 axis is given by (45) and from the Sommerfeld condition this may be equalized as:

This let us write the following scheme:

|  |  |
| --- | --- |
|  | (49) |

Now suppose that we want to write a scheme for the east most point of our region. From the central scheme (48) we ignore the value of but we may now replace it by its new expression from (49) and obtain the scheme written for the east side in Table 4.

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: . Therefore the Sommerfeld condition may be written:

We then sum two version of equation (42) in its two dimensional version, one at constant and the other at constant and obtain:

Now the Sommerfeld condition may be written:

=

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

And if we replace this second order derivative expression in (33) we obtain the scheme version of the Helmholtz equation:

And the last equation let us find directly the scheme given in Table 4 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.

## Class model of the framework

### Central Scheme Module

### Sommerfeld Scheme Module

### Simulation Module

### Reporting Module

Template for equation

|  |  |  |
| --- | --- | --- |
|  |  | (50) |

1. [http://www.sdms.org](http://www.sdms.org/public/soundmedicine.asp), Society of Diagnostic Medical Sonography. [↑](#footnote-ref-2)
2. “Detection and characterization of breast masses with ultrasound tomography: Clinical results”,

   Neb Duric, Peter Littrup, Cuiping Li, Olsi Rama, Lisa Bey-Knight, Steven Schmidt and Jessica Lupinacci

   Medical Imaging 2009: Ultrasonic Imaging and Signal Processing, edited by Stephen A. McAleavey,

   Jan D'hooge, Proc. of SPIE Vol. 7265, 1-8 [↑](#footnote-ref-3)
3. Informally, as if there exist and such that for . If as as if there exist and such that for . [↑](#footnote-ref-4)
4. 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 that gives the coefficient of the matrix and that take the Dirichlet value is placed in the vector thus for more details about this technique see [[4](#Cha10)], **[**[5](#Bur10)**]** or [[3](#LeV07)]. [↑](#footnote-ref-5)