Optimal Finite Difference Schemes
for Wave Equation

By

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CIIT/FA10-MSMATH-011/LHR

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Declaration

I Hifza Iqbal with registration number **CIIT/FA10-MSMATH-011/LHR** hereby declare that I have produced the work presented in this thesis, during the scheduled period of study. I also declare that I have not taken any material from any source except referred to wherever due, that amount of plagiarism is within acceptable range. If a violation of HEC rules on research has occurred in this thesis, I shall be liable to punishable action under the plagiarism rules of the HEC.

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It is certified that Hifza Iqbal & CIIT/FA10-MSMATH-011/LHR has carried out all the work related to this thesis under my supervision at the Department of Mathematics, COMSATS Institute of Information Technology, Lahore campus and the work fulfills the requirement for award of MS degree.

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To my Father M. Iqbal,
Mother Nusrat Shahida,
sister Shaista Iqbal,
brothers M. Hamza Bilal,
M. Mohsin Bilal
and all Teachers.

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Abstract

In this research work the novel optimal central finite difference schemes for solving the transient wave equation, are developed and analyzed. The novel schemes (a) give exact value at the nodes of the grid, meaning that an exact solution is possible for the transient wave equation; (b) the key advantage is that they have the simple structure as that of the standard central finite difference schemes, so we just need to make few amendments in the standard codes, instead of writing the new codes altogether; (c) above all, the beauty lies in the fact that they do not require fine mesh size and works for any wave number, specially for high wave number. Finally, in order to display the actual power of the novel schemes, numerical computations and graphical representations for two model problems are added, by using both novel and standard central finite difference schemes, which support our theoretical results, by showing the superiority of the novel schemes compared to the standard schemes.

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Introduction

1.1 Motivation and Introduction

Our holy book THE QURAN invites every single human being to observe the creation of this universe so that at the same time he can praise the creator as well as learn to benefit himself from this ever changing world. There are many phenomena in nature, which occur over finite (or infinite) regions of space and time, can be described in terms of properties that exist at each point of space and time separately. This manner of making the nature comprehensible is extended from a single point particle motion to the complex; which can be in the form of gases, fluids, solids, light, heat, electricity etc. When we try to think of mathematics (model) associated with a natural phenomena we end up with an equation relating independent, dependent variables, changes of dependent with respect to independent variables, and influencing parameters. Simplest of these equations are algebraic equations and complex ones are differential equations. The differential equations are the mathematician's foremost aid to describe the change. Interestingly, in recent decades with the efforts of many the subject has experienced a vigorous growth and the research is marching on at a brisk pace, because of its role in making human lives much easier, better and secure. Hence, to describe the phenomenal change we need to formulate a differential equation and then even-

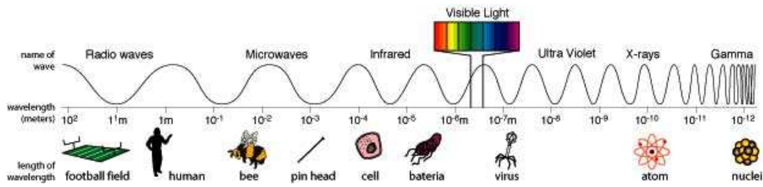

Figure 1.1: Waves of different wave lengths.

tually solving that differential equation for the purpose of predicting measurable properties of the phenomenon.

It would not be wrong to say that our curiosity and needs pushes us to explore and create new things, and the nature is there to teach us at the route of knowledge and innovation. For instance; when we learned about the defensive system of a fly we invented the radars, antennas, similarly when human saw the birds flying, it gave birth to the aeroplanes. We observed how the dolphins communicate with each other and find their path under water with the help of sound waves, so we developed our submarines on that mechanism, these are just few examples from the nature. All these devices work on the wave propagation phenomena hence, it is not surprising that wave propagation phenomena occurs frequently in various walks of humans covering their domestic, social and medical, industrial as well as security needs. Following are common examples humans encounter on daily basis in present era such as mobiles, ultrasound scans, microwave ovens, television, radio, radars and satellites. Whereas industrial based applications of wave propagation fall in specialized fields such as acoustics, electromagnetic and geophysics etc [1, 2, 3, 7, 8, 9, 16, 17, 18, 19, 20, 29, 30, 35, 39, 40].

We now introduce ourselves about how radar propagation works [11], which is a very common example of wave propagation phenomenon.

- Duplexer switches magnetron through to antenna;
- Antenna acts as transmitter, sending narrow beam of radio waves through the air;

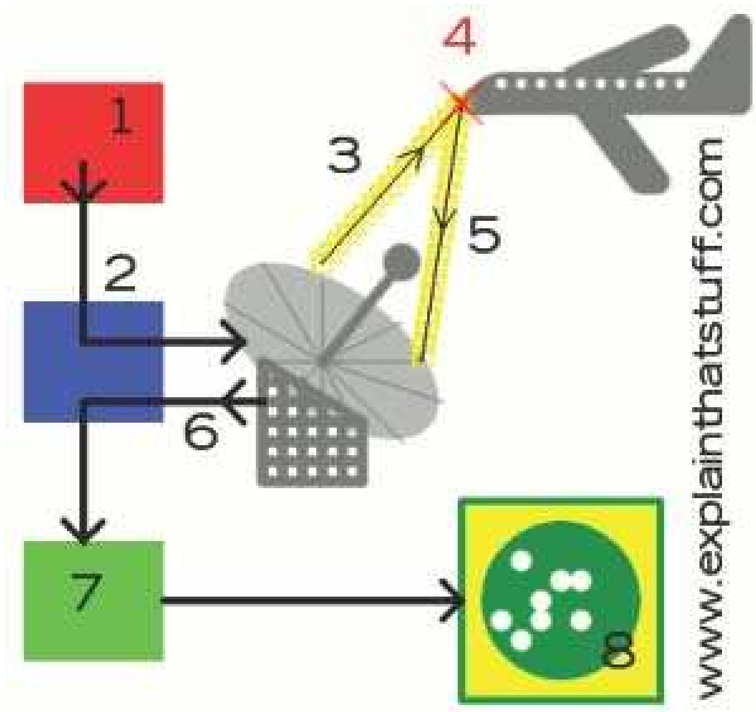

Figure 1.2: Working of a radar.

- Radio waves hit enemy air plane and they reflect back;
- Antenna picks up reflected waves during a break between transmissions;
- Duplexer switches antenna through to receiver unit;
- Computer in receiver unit processes reflected waves and draws them on a television screen;
- Enemy plane shows up on television radar display with any other nearby targets.

Before moving towards the main topic of this thesis which is computational wave propagation, we first review some basic definitions.

1.2 Differential equation

The role of differential equations in mathematics and other sciences have become increasingly significant. There are lots of applications and related fields of differential equations like in general mathematics, topological groups, functions of complex variables, potential theory, several complex variables and analytic space, ordinary differential equation, finite differences and functional equations, fourier analysis, functional analysis, operator theory, calculus of variations and optimal control, differential geometry, global analysis, analysis of manifolds probability theory and stochastic process, numerical analysis, mechanics of solids, fluid mechanics, optics, electromagnetic theory, classical thermodynamics, heat transfer, quantum theory, statistical mechanics, structure of matter, relativity and gravitational theory, geophysics, biology and other natural sciences, system theory; control etc [11].
Mathematically we say that if an equation involves a dependent variable and its derivatives with respect to one or more independent variables then it is known as a differential equation. For instance, lets take a look at two examples of differential equations from the real world;

1. Newton's second law of motion :

   This fundamental law states that the net force F applied to some body produces a proportional acceleration a *(dv/dt)*. Refereing that we have the following differential equation,

   $$F = m\frac{dv}{dt} \qquad \text{where m>0, is mass of the body.}$$

2. Newton's law of cooling :

   The law states that the time rate of change of the temperature of a body in the given environment is proportional to the difference between the temperature T of the body and the temperature T_0 of the surrounding environment. It gives the following differential equation,

   $$\frac{dT}{dt} = k(T - T_0). \qquad \text{where k>0, constant of propostionality.}$$

Similarly, the following equations also govern some physical phenomena, one can see the detail in [11].

$$\frac{d^2u}{dx^2} + x\frac{du}{dx} = 0, \tag{1.1}$$

$$\frac{d^2u}{dx^2} = -kx, \tag{1.2}$$

$$x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} = nx, \tag{1.3}$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = mx. \tag{1.4}$$

These were few examples of differential equations. Which can further be characterized as:

- Ordinary differential equation,
- Partial differential equation.

Each is defined in literature as follows.

1.2.1 Ordinary differential equation

An ordinary differential equation (ODE) is an equation that involves an unknown function (the dependent variable) and some of its derivatives with respect to a single independent variable. An nth order equation has the highest order derivative of order n. Examples are given in (1.1) and (1.2).

1.2.2 Partial differential equation

A partial differential equation (PDE) is an equation that involves an unknown function (the dependent variable) and some of its derivatives with respect to more than one independent variables. Examples are given in (1.3) and (1.4).

Terrifying though they may sound, these equations are bread and butter objects for any one who uses maths to solve real life problems. This is because these equations describe change, and change is what characterizes most things in the world:

motion is a change in position over time, growth is a change in size over time, etc. Mathematical descriptions of physical systems are therefore typically phrased in terms of rates of change, so derivatives in maths represent some meaning. Differential equations relate physical variables like mass, energy and velocity to their variation with respect to more elementary variables like time and position. Since, a differential equation is an equation involving the derivatives of a function, and thus solving it amounts to finding the function itself.
In the upcoming section, we will see how and on what grounds the two dimensional second order partial differential equations are classified.

1.3 Special cases of two dimensional second order PDE

In general, the two dimensional second order PDE is given by, [11]

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu + g = 0 \tag{1.5}$$

Where a, b, c, d, e, f and g can be the functions of independent variables x, y and of dependent variable u. Equation (1.5) mostly occurs than others and describe different physical phenomena depending on the values of a, b, c, d, e, f and g. Few are listed in Table 1.1, according to the following criteria.
The equation (1.5) is said to be *elliptic* if $b^2 - 4ac < 0$, *parabolic* if $b^2 - 4ac = 0$, and *hyperbolic* if $b^2 - 4ac > 0$.

As we said earlier, that the wave propagation phenomena is playing a vital role in science and information technology. Therefore, the next section is devoted to give the reader an understanding about what do we mean by waves and what properties they possess.

Heat Equation−parabolic (diffusive or dispersive)	$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$
Wave Equation−hyperbolic (propagating signals, vibrations)	$\frac{\partial^2 u}{\partial^2 t} = c^2\frac{\partial^2 u}{\partial x^2}$
Laplace Equation−elliptic (fluids)	$\frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial y^2} = 0$

Table 1.1: Common PDE's classification

1.4 Wave and its properties

Since, computational wave propagation is the central topic of this thesis, but before delving into mathematical details, in this section we will learn about the physics of waves and its properties. Generally, wave is a disturbance that travels through space and time, usually accompanied by the transfer of energy (information) over large distances, which has simple mathematical form given in the above Table 1.1. The best demonstration for this is the Mexican wave, which is an example of metachronal rhythm, that is achieved in a packed stadium when successive groups of spectators stand slowly by stretching their arms and return to their seats. Resulting a wave, and it travels through the crowd, yet not a single person moved away from the seat [11]. Next, we will see the properties of waves propagating in an isotropic materials such as steel and aluminum;

1.4.1 Phase velocity (v_p)

The phase velocity of the wave is defined as the rate at which the phase of the wave propagates in the space. Mathematically, it is the ratio of angular frequency

Figure 1.3: Mexican wave

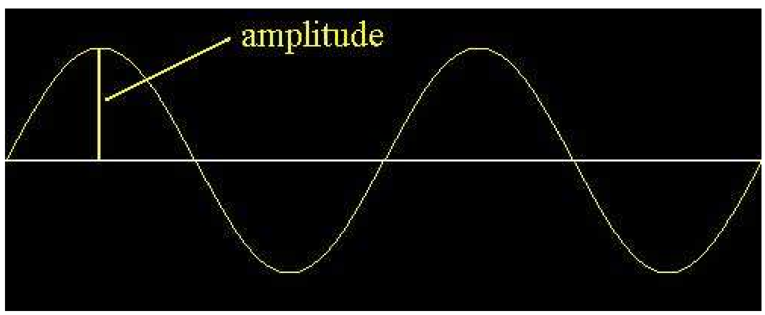

Figure 1.4: Amplitude.

ω and the wavenumber k, that is

$$v_p = \frac{\omega}{k}.$$

If we take out the direction, then it is the speed (c) of propagation. The SI unit of measurment is meter per second.

1.4.2 Amplitude(A)

The wave's amplitude is defined, as the maximum magnitude of the displacement of wave, from its equilibrium position. It is measured in SI unit of meter.

1.4.3 Frequency(f)

Frequency of the wave is the number of cycles in a unit of time. The SI units of frequency is the hertz (Hz) and 1Hz=1 cycle/s=1/s.

1.4.4 Angular frequency(ω)

It is denoted by ω, and defined as 2π times the frequency, with SI unit of measurement, radians per second.

$$\omega = 2\pi f = \frac{2\pi}{T} \quad \text{or} \quad \omega = ck.$$

1.4.5 Period(T)

The wave period is defined as the time required to complete one wave cycle or in other words it is the time taken by the wave to travel from crest to crest or trough to trough. Its SI unit of measurement is second (though it may be referred to as seconds per cycle).

$$T = \frac{1}{f} = \frac{2\pi}{\omega}.$$

1.4.6 Wavelength(λ)

The wave length is denoted by λ, and defined as the distance between two sequential crests or troughs. Mathematically, we calculate it as follows.

$$\lambda = \frac{2\pi}{k}.$$

The SI unit of measurement is meter. We also have the following expression for λ in terms of speed and frequency of the wave

$$\lambda = \frac{c}{f},$$

which shows that the wavelength is directly proportional to the speed of the wave and inversely proportional to the frequency of the wave.

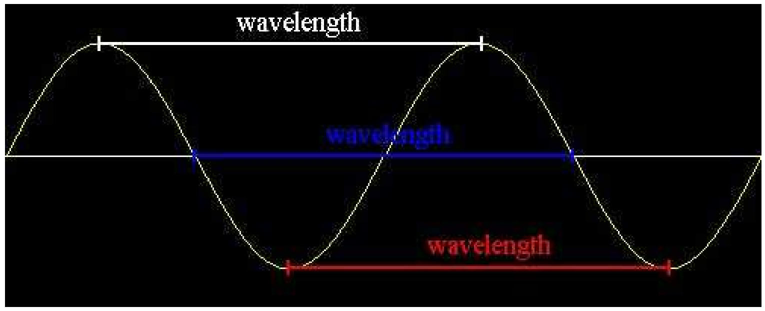

Figure 1.5: Wavelength.

1.4.7 Wavenumber(k)

The wavenumber is also known as the propagation constant, this useful quantity is defined as the ratio of 2π and the wave length. The SI unit of measurement is radians per meter.

$$k = \frac{2\pi}{\lambda} \quad \text{or} \quad k = \frac{\omega}{c}.$$

1.4.8 Pulse

A pulse of wave is defined as one half-wavelength, from equilibrium position of wave.

1.5 The wave equation

Mathematically, wave propagation phenomena can be represented either by an ordinary differential equation or by a partial differential equation. For instance, consider the acoustic pressure $u(x, t)$ of sound waves propagating in a homogeneous isotropic medium having speed, c. Reconsider the wave equation we defined in Table 1.1, that is

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \qquad \text{where u=u(x,t).} \tag{1.6}$$

This is known as one dimensional, transient wave equation [11, 16, 17, 35, 37, 40]. The key usefulness of this equation is that, whenever it occurs we know that the function $u(x,t)$ acts as a wave having the propagation speed c, and therefore the situation can be described by using the wave function. The general solution of (1.6) is,

$$u(x) = Ae^{i(kx-\omega t)} + Be^{-i(kx-\omega t)}$$

where A, B $\in \mathbb{C}$ are a set of constants to be determined, for this we need the boundary conditions. In order to remove the complexity of analysis the transient (time dependent) wave equation can be converted into a time harmonic form (time independent), by using the following substitution.

$$u(x,t) = u(x)e^{i\omega t}, \qquad \text{where } \omega > 0 \tag{1.7}$$

when (1.7) is twice partially differentiated, with respect to $'x'$ and $'t'$ gives,

$$\frac{\partial^2 u}{\partial x^2} = e^{i\omega t}u''(x)$$

$$\text{and} \qquad \frac{\partial^2 u}{\partial t^2} = -\omega^2 u''(x)e^{i\omega t}.$$

Inserting the values of $\partial^2 u/\partial x^2$ and $\partial^2 u/\partial t^2$ in equation (1.6), we get after simplification.

$$u''(x) + k^2 u(x) = 0, \qquad \text{where k=}\omega\text{/c>0.} \tag{1.8}$$

The above equation (1.8) is known as *time independent*, *time harmonic*, *reduced* or *scalar* wave equation. Furthermore, it is named as *Helmholtz equation* [1, 2, 3, 7, 8, 9, 10] and have the general solution of the following form.

$$u(x) = Ae^{ikx} + Be^{-ikx} \tag{1.9}$$

where A, B $\in \mathbb{C}$ are a set of constants to be determined, which again requires the use of boundary conditions. Whereas, the two dimensional form of Helmholtz equation is

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} + k^2 u(x,y) = 0. \tag{1.10}$$

Similarly, the two dimensional transient wave equation has the form,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \qquad \text{where u=u}(\mathbf{x}) \text{ with } \mathbf{x}\text{=(x,y,t)}$$

and the three dimensional Helmholtz equation is

$$\frac{\partial^2 u(x,y,z)}{\partial x^2} + \frac{\partial^2 u(x,y,z)}{\partial y^2} + \frac{\partial^2 u(x,y,z)}{\partial z^2} + k^2 u(x,y,z) = 0.$$

in the same way, the three dimensional transient form of the wave equation is given by,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \qquad \text{where u=u}(\mathbf{x})\text{, with } \mathbf{x}\text{=(x,y,z,t).}$$

As we said earlier that without consistent initial conditions and most importantly the boundary conditions, we cannot solve a problem. So, in the next section we will have a look at frequently used boundary conditions for wave propagation problems.

1.6 Boundary conditions

Whenever we model a real world phenomena, it consist of an ordinary (or partial) differential equation or a system of ordinary (or partial) differential equation with a set of constraints for the boundary known as boundary conditions. Before we tackle with our actual problem, we allocate this section to the study of boundary conditions widely used in the literature of computational wave propagation.

1.6.1 Different types of boundary conditions

The boundary conditions depending upon their nature can be divided into four types [11]:

1. Dirichlet boundary conditions;
2. Neuman boundary conditions;
3. Mixed boundary conditions;
4. Robin or non reflecting boundary conditions.

Each can be described as follows:

1.6.2 Dirichlet boundary conditions

It is the first type of boundary condition and gives us the functional value at the boundary. When we are dealing with ordinary differential equation (1.8), the Dirichlet boundary conditions defined in domain $[a, b]$, have the form

$$u(a) = \alpha \qquad \text{and} \quad u(b) = \beta$$

where $\alpha, \beta \in \mathbb{C}$ are arbitrary constants.

But when we are dealing with partial differential equation (1.10), the Dirichlet boundary conditions defined on a rectangular domain $[0, a] * [0, b]$ with $u = u(x, y)$ have the form,

$$u = \begin{cases} \alpha_0(x) \text{ along } y = 0, \text{with } 0 \le x \le a \\ \beta_b(x) \text{ along } y = b, \text{with } 0 \le x \le a \\ \alpha_0(y) \text{ along } x = 0, \text{with } 0 \le y \le b \\ \beta_a(y) \text{ along } x = a, \text{with } 0 \le y \le b \end{cases}$$

1.6.3 Neuman boundary conditions

It is the second type of boundary condition and gives the normal derivative value at the boundary. In case of ordinary differential equation (1.8) the Neuman boundary conditions defined in domain $[a, b]$ are given as

$$u'(a) = \alpha \qquad \text{and} \quad u'(b) = \beta$$

where $\alpha, \beta \in \mathbb{C}$ are arbitrary constants.

Whereas, in case of partial differential equation (1.10) this kind of boundary conditions defined on a rectangular domain $[0, a] * [0, b]$ with $u = u(x, y)$ can be written in the form as,

$$
\begin{aligned}
-\frac{\partial u}{\partial x} &= \psi(0,y) \ \text{ along } \ x=0, \text{with } \ 0 \leq y \leq b \\
\frac{\partial u}{\partial x} &= \psi(a,y) \ \text{ along } \ x=a, \text{with } \ 0 \leq y \leq b \\
-\frac{\partial u}{\partial y} &= \psi(x,0) \ \text{ along } \ y=0, \text{with } \ 0 \leq x \leq a \\
\frac{\partial u}{\partial y} &= \psi(x,b) \ \text{ along } \ y=b, \text{with } \ 0 \leq x \leq a
\end{aligned}
$$

where the direction of $\partial u/\partial x$ and $\partial u/\partial y$ are those of increasing x and y; the minus sign is attached, where appropriate, in order to ensure that all the normal derivatives are directed outwards.

1.6.4 Mixed boundary conditions

When dealing with mixed boundary conditions the domain is divided into different regions and then at one boundary the first type of boundary condition is applied, whereas, on the other boundary the second type of boundary condition is applied, or vice versa. For ordinary differential equation (1.8), the mixed boundary conditions are of the following form, by taking Dirichlet boundary condition at the left end a of $[a, b]$ domain and Neuman boundary condition at right end b, for the same $[a, b]$ domain.

$$u(a) = \alpha \qquad \text{and} \qquad u'(b) = \beta$$

where $\alpha, \beta \in \mathbb{C}$ are arbitrary constants.

Similarly, in case of partial differential equation (1.10), the mixed boundary conditions defined on a rectangular domain $[0, a] * [0, b]$ with $u = u(x, y)$ can be defined as,

$$\begin{aligned} u &= \alpha_0(x,0) \ \text{ along } \ y=0, \ \text{ with } \ 0 \le x \le a \\ u &= \alpha_0(0,y) \ \text{ along } \ x=0, \ \text{ with } \ 0 \le y \le b \\ \frac{\partial u}{\partial x} &= \phi(a,y) \ \text{ along } \ x=a, \ \text{ and } \ 0 \le y \le b \\ \frac{\partial u}{\partial y} &= \phi(x,b) \ \text{ along } \ y=b, \ \text{ and } \ 0 \le x \le a \end{aligned}$$

here, we have applied the Dirichley boundary conditions at $x = 0$ and $y = 0$, whereas the Neuman boundary conditions at $x = a$ and $y = b$.

1.6.5 Robin or Non−reflecting boundary conditions

Also named as radiating, absorbing, silent, transmitting, transparent, open, free−space and one−way boundary conditions [5]. The Non−reflecting boundary conditions are defined as a linear combination of Dirichlet and Neuman boundary condition, and are for the scattering problems, [5,31]. For ordinary differential equation (1.8) the non−reflecting boundary conditions are of the following form, in the domain $[a, b]$

$$\alpha_1 u(a) + \beta_1 u'(a) = \gamma_1$$
$$\alpha_2 u(b) + \beta_2 u'(b) = \gamma_2$$

where $\alpha_i, \beta_i, \gamma_i \in \mathbb{C}$, for i=$1, 2$ are arbitrary constants to be determined.

In case of partial differential equation (1.10), the non−reflecting boundary conditions defined on a rectangular domain $[0, a] * [0, b]$ with $u = u(x, y)$ can be defined as,

$$
\begin{aligned}
-\frac{\partial u}{\partial x} + \alpha_0 u = \gamma_0(y), \quad 0 \le y \le b \\
\frac{\partial u}{\partial x} + \alpha_a u = \gamma_a(y), \quad 0 \le y \le b \\
-\frac{\partial u}{\partial y} + \beta_0 u = \delta_0(x), \quad 0 \le x \le a \\
\frac{\partial u}{\partial y} + \beta_b u = \delta_b(x), \quad 0 \le x \le a
\end{aligned}
$$

along $x = 0$, $x = a$, $y = 0$, $y = b$, respectively. Whereas, the quantities α_0, α_b, β_0, β_a are real valued and they can be positive, negative and zero. In the above defined Robins boundary conditions the directions of $\partial u/\partial x$ and $\partial u/\partial x$ are taken to have positive increase along x and y direction and the negative sign is attached to make sure that each normal derivative to ∂R is directed away from the interior of R.

1.7 Examples of wave propagation problems

This section is included in the text for the clear understanding, about the effects of different types of boundary conditions, on the wave propagation problems. The following examples will help us to observe the difference in wave function u, in two ways. The first case is when we change the value of boundary condition but keeping the same type of boundary condition, and the second case is when we change the type of boundary condition. The biggest advantage of this topic is that, we have the variety of solutions, since at the same time one can witness the solution of one dimensional time independent wave equation as well as the solution of one dimensional time dependent wave equation. So, lets begin with (1.8), that is

$$
u''(x) + k^2 u(x) = 0, \qquad \text{where x} \in \text{(0,1)}.
$$

Since, we require non-trivial, exact solution of the O.D.E and it can also be calculated with the help of method already present in the literature [4, 35, 40].

The characteristic equation of (1.8) is

$$D^2 + k^2 = 0 \Longrightarrow D = \pm ik.$$

Hence, the general solution is of the form

$$u(x) = Ae^{ikx} + Be^{-ikx} \tag{1.11}$$

where A, B $\in \mathbb{C}$ are unknown arbitrary constants. Now, to find the particular solution of the above problem we will make use of different types of boundary conditions.

1.7.1 Particular solution with Dirichlet boundary conditions

First of all, consider the following Dirichlet boundary conditions;

$$u(0) = 1 \quad \text{and} \quad u(1) = e^{-ik}.$$

Next, apply the boundary conditions on the solution (1.11), we have the following two equations.

$$\begin{aligned} A + B &= 1 \\ Ae^{ik} + Be^{-ik} &= e^{-ik}. \end{aligned}$$

Simultaneously solving these equations we have

$$A = 0 \text{ and } B = 1.$$

Substitute the value of A and B in (1.11), we get

$$u(x) = e^{-ikx}.$$

If we multiply both sides by $e^{i\omega t}$, we get the transient wave solution for (1.6) as ,

$$u(x,t) = e^{-i(kx-\omega t)}.$$

Secondly, if we use the following Dirichlet boundary conditions;

$$u(0) = 0 \quad \text{and} \quad u(1) = 1,$$

we have different value of A and B, that is

$$A = \frac{1}{2i\sin(k)} \quad \text{and} \quad B = -\frac{1}{2i\sin(k)}.$$

After inserting the value of A and B, we have the solution of (1.8) as follows;

$$u(x) = \frac{\sin(kx)}{\sin(k)}.$$

The corresponding solution of (1.6) is,

$$u(x,t) = \left[\frac{\sin(kx)}{\sin(k)}\right](\cos(\omega t) + i\sin(\omega t)).$$

It is obvious that, even when we change the values of the same type of boundary conditions we have a different solution for (1.8) and (1.6).

1.7.2 Particular solution with Neuman boundary conditions

This time we solve (1.8), along with the following Neuman boundary conditions.

$$-u'(0) = ik \quad \text{and} \quad u'(1) = -ike^{-ik}.$$

The first derivative of (1.9) is,

$$u'(x) = ikAe^{ikx} - ikBe^{-ikx}.$$

Next, applying $u'(x)$ on the boundary, we get the following two equations.

$$\begin{aligned} -A + B &= 1 \\ ikAe^{ik} - ikBe^{-ik} &= -ike^{-ik}. \end{aligned}$$

Simultaneously solving these equations we have

$$A = 0 \text{ and } B = 1.$$

Substitute the value of A and B in (1.11), we get

$$u(x) = e^{-ikx}.$$

If we multiply both sides by $e^{i\omega t}$, we get the transient wave solution for (1.6) as,

$$u(x,t) = e^{-i(kx-\omega t)}.$$

These solutions are same as we calculated with first type of Dirichlet boundary conditions. Secondly, if we use the following Neuman boundary conditions,

$$-u'(0) = 0 \quad \text{and} \quad u'(1) = 1,$$

we have the following values of A and B,

$$A = B = -\frac{1}{2k\sin(k)}.$$

After inserting the values of A and B we have the solution of (1.8) as follows;

$$u(x) = -\frac{\cos(kx)}{k\sin(k)}.$$

The corresponding solution of (1.6) is,

$$u(x,t) = -\left[\frac{\cos(kx)}{k\sin(k)}\right](\cos(\omega t) + i\sin(\omega t)).$$

1.7.3 Particular solution with mixed boundary conditions

Reconsider (1.8), along with the following mixed boundary conditions.

$$u(0) = 1 \quad \text{and} \quad u'(1) = -ike^{-ik}.$$

Apply the boundary conditions on the solution (1.11), along with its first derivative, then we have the following two equations.

$$\begin{aligned} A + B &= 1 \\ ikAe^{ik} - ikBe^{-ik} &= -ike^{-ik}. \end{aligned}$$

Simultaneously solving these equations we have

$$A = 0 \text{ and } B = 1.$$

Substitute the value of A and B in (1.11) equation, we get

$$u(x) = e^{-ikx}.$$

If we multiply both sides by $e^{i\omega t}$, we get the transient wave solution for (1.6) as ,

$$u(x,t) = e^{-i(kx-\omega t)}.$$

These above two solutions are again the same which we computed by using first kind of Dirichlet and then by Neuman boundary conditions.
Similarly, if we use the following Mixed boundary conditions,

$$u(0) = 0 \quad \text{and} \quad u'(1) = 1,$$

we have,

$$A = \frac{1}{2ik\cos(k)} \quad \text{and} \quad B = -\frac{1}{2ik\cos(k)}.$$

After inserting the values of A and B we have the solution of (1.8) as follows;

$$u(x) = \frac{\cos(kx)}{k\sin(k)}.$$

The corresponding solution of (1.6) is,

$$u(x,t) = \left[\frac{\sin(kx)}{k\cos(k)}\right](\cos(\omega t) + i\sin(\omega t)).$$

1.7.4 Particular solution with non−reflecting boundary conditions

Solving (1.8), along with the non−reflecting boundary conditions defined below,

$$-u'(0) - iku(0) = 0 \quad \text{and} \quad u'(1) - iku(1) = -2ike^{-ik}.$$

Apply the boundary conditions on the solution (1.11) along with its first derivative, we have the following values of A and B.

$$A = 0 \text{ and } B = 1.$$

Substitute the value of A and B in (1.11) equation, we get

$$u(x) = e^{-ikx}.$$

If we multiply both sides by $e^{i\omega t}$, we get the transient wave solution for (1.6) as,

$$u(x,t) = e^{-i(kx-\omega t)}.$$

These solutions are again the same as we computed in first type of Dirichlet, Neuman, and Mixed boundary conditions.

Similarly, if we use the following non$-$reflecting boundary conditions,

$$-u'(0) + iku(0) = 0 \quad \text{and} \quad u'(1) + iku(1) = 1.$$

we get different values of A and B, that is

$$A = \frac{1}{2ike^{ik}} \quad \text{and} \quad B = 0.$$

After inserting the values of A and B we have the solution of (1.8) as follows;

$$u(x) = \frac{e^{ikx}}{2ike^{ik}}.$$

The corresponding solution of (1.6) is,

$$u(x,t) = \left[\frac{e^{i(kx+\omega t)}}{2ike^{ik}}\right].$$

From this exercise, we can easily comprehend that, for the same problem, by using different types of boundary conditions we have different solutions. Consequently, boundary conditions play a vital role in defining the problem. Moving forward, before we look into the numerical dispersion and dissipation which is the central topic of this thesis, first we will see that what dispersive and non-dispersive, dissipative and non-dissipative waves are?

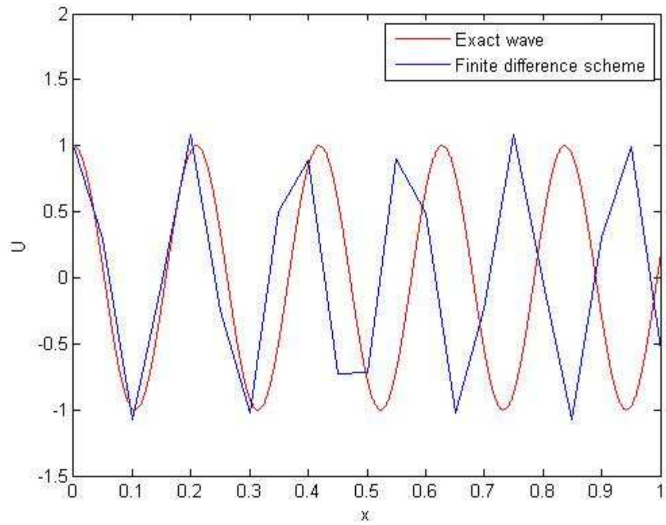

Figure 1.6: Dispersion in Helmholtz equation with $k = 30$, and $N = 20$.

1.8 Dispersive and Non dispersive waves

A wave is defined to be dispersive if its phase velocity depends on the frequency or equally on the wavenumber, otherwise the wave is defined to be non dispersive [1, 2, 6, 12, 14, 16, 17, 21, 24, 26, 27, 28, 35, 40]. Well, in order to have a clear understanding lets see an example. Reconsider equation (1.6),

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}.$$

Since, we want to have a plane wave solution of the form $u(x,t) = e^{i(kx-\omega t)}$, differentiating twice this $u(x,t)$ with respect to x and t, we have $\frac{\partial^2 u}{\partial x^2} = -k^2 u(x,t)$ and $\frac{\partial^2 u}{\partial t^2} = \omega^2 u(x,t)$. Insert these values in (1.6), we get

$$\omega^2 = c^2 k^2 \quad \Rightarrow \quad \omega = \pm ck. \tag{1.12}$$

As the phase velocity is defined by the relation; $v_p = \frac{\omega}{k}$. Insert the value of ω, from (1.12), into the expression of v_p, we get $v_p = \pm c$, this proves that the phase velocity of the wave is independent of frequency as well as from the wavenumber. Hence, the wave equation (1.6), is non dispersive.

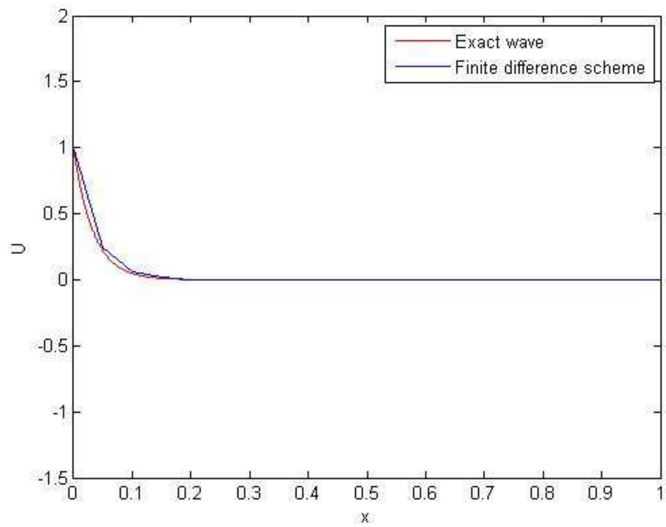

Figure 1.7: Dissipation in Helmholtz equation with $k = 30i$, and $N = 20$.

Few authors define the dispersion in a different way. They say that, if the waves of different wavelengths propagate at different phase velocities then they are said to be dispersive, otherwise non−dispersive. In Figure 1.6, the dispersion is clearly visible as the numerical wave is lagging behind through out the interval compared with the exact wave.

1.9 Dissipative and Non dissipative waves

If the wavenumber k is complex i.e;

$$k = k_r + ik_c \in \mathbb{C}$$

with k_r and $k_c \in \mathbb{R}$, and $k_c \neq 0$ then $k \in \mathbb{C}$, in this situation, it is said that the wave is dissipative. Otherwise, if $k_c = 0$ then $k \in \mathbb{R}$, it shows that the wave is non dissipative. For instance, by considering (1.12) we computed, $k = \pm\dfrac{\omega}{c} \in \mathbb{R}$, as k is real, therefore the wave equation (1.6) is non dissipative.

It is widely proven that, when the same wave equation which is neither dispersive nor dissipative is solved by using numerical schemes, manifest both numerical dispersion and numerical dissipation because of the discrete nature of these numerical schemes. One can avoid the numerical dissipation by imposing the restriction on k as it should $\in \mathbb{R}$. Whereas, to bypass the numerical dispersion, is not an easier task, it demands lots of effort and time. So, we devote the following section to study in detail the numerical dispersion. If one needs more detail about the dispersion and dissipation, it can be found in [6, 35]. Figure 1.7, displays the dissipation of a wave.

1.10 Numerical dispersion

Since, we can control the dissipation by choosing $k \in \mathbb{R}$, and so the problem remains to control or to remove the dispersion. Now, we know the meaning of dispersion and it displays a particular behavior as a phase lead or a phase lag of the wave [12, 13, 14, 15, 24, 26]. In practice, it is assumed that the dispersion arises because the numerical wave and an exact wave are propagating with different phase velocities, since the waves have different wave number. So, we start this section with the definition of numerical dispersion, which is defined as a ratio of continuous propagation speed (c) and discrete propagation speed ($\tilde{c}$). i.e;

$$\begin{aligned} dispersion &= \frac{c}{\tilde{c}} \\ \text{or it can be written as} &= \frac{\tilde{k}}{k}. \end{aligned}$$

As we know that $c = \dfrac{\omega}{k}$ and take $\tilde{c} = \dfrac{\omega}{\tilde{k}}$.
If $\dfrac{\tilde{k}}{k} = 1$, which is an ideal situation implies that, $\tilde{k} = k$ or $\tilde{k} - k = 0$, meaning that there is no dispersion in the numerical scheme.
However, if $\dfrac{\tilde{k}}{k} \neq 1$ then we have,

$$\frac{\tilde{k}}{k} = 1 \pm (error)$$

$$\tilde{k} = k \pm k(error)$$

$$\tilde{k} - k = \pm k(error).$$

In the upcoming sections, we will see the arbitrary order finite difference approximations for the second order derivative, and then later on, by using these approximations we will construct different order central finite difference schemes for the Helmholtz equation. Furthermore, we will observe the dispersion relation for these numerical schemes.

1.11 Central finite difference approximations for second order derivative

By the aid of Taylor's series, different central finite difference approximations are constructed for second order derivative, in the following manner [4, 6, 16, 17, 35, 40].

1.11.1 Second order central finite difference approximation

Lets start by constructing second order central finite difference approximation of second order derivative. Consider the Taylor's series approximations of $u(x+h)$ and $u(x-h)$, given by

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \frac{h^4}{4!}u^4(x) + \cdots$$

and

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2!}u''(x) - \frac{h^3}{3!}u'''(x) + \frac{h^4}{4!}u^4(x) + \cdots .$$

As we need second order approximation of $u''(x)$, so by adding the above two equations, we get

$$\begin{aligned} u(x+h) + u(x-h) &= 2u(x) + h^2u''(x) + \frac{h^4}{12}u^4(x) + \cdots \\ \text{or} \qquad \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} &= u''(x) + O(h^2). \end{aligned}$$

Hence,

$$u''(x) \approx \frac{1}{h^2}[u(x+h) - 2u(x) + u(x-h)]. \tag{1.13}$$

This is the required *second order central finite difference approximation of* $u''(x)$, [11, 16].

1.11.2 Fourth order central finite difference approximation

Above we constructed the second order central finite difference approximation of $u''(x)$ with the help of Taylor's series of $u(x+h)$ and $u(x-h)$. Now, to get forth order central finite difference approximation, we need to introduce two additional nodes in the grid that is, $(x+2h)$ and $(x-2h)$.

Thus, the Taylor's series approximations of $u(x+2h)$ and $u(x-2h)$ are given by,

$$u(x+2h) = u(x)+2hu'(x)+2^2\frac{h^2}{2!}u''(x)+2^3\frac{h^3}{3!}u'''(x)+2^4\frac{h^4}{4!}u^4(x)+2^5\frac{h^5}{5!}u^4(x)+\cdots$$

and

$$u(x-2h) = u(x)-2hu'(x)+2^2\frac{h^2}{2!}u''(x)-2^3\frac{h^3}{3!}u'''(x)+2^4\frac{h^4}{4!}u^4(x)-2^5\frac{h^5}{5!}u^4(x)+\cdots.$$

By adding the above two equations, we get

$$\begin{aligned} u(x+2h)+u(x-2h) &= 2u(x)+4h^2u''(x)+\frac{4}{3}h^4u^4(x)+\cdots \\ \text{or} \quad \frac{u(x+2h)-2u(x)+u(x-2h)}{4h^2} &= u''(x)+\frac{1}{3}h^2u^4(x)+\cdots. \end{aligned}$$

To achieve the required order, we have to solve the linear combination of the following two equations,

$$\left[\frac{u(x+h)-2u(x)+u(x-h)}{h^2}\right] = u''(x)+\frac{h^2}{12}u^4(x)+\frac{h^4}{360}u^6(x)+\cdots \tag{1.14}$$

and

$$\left[\frac{u(x+2h)-2u(x)+u(x-2h)}{4h^2}\right] = u''(x)+\frac{1}{3}h^2u^4(x)+\frac{2}{45}h^4u^6(x)+\cdots. \tag{1.15}$$

To write a linear combination, multiply equation (1.14) by A_1 and (1.15) by A_2, then add. We get,

$$A_1\left[\frac{u(x+h)-2u(x)+u(x-h)}{h^2}\right]+A_2\left[\frac{u(x+2h)-2u(x)+u(x-2h)}{4h^2}\right]$$

$$\begin{aligned}
&= A_1u^2(x)+A_1\frac{h^2}{12}u^4(x)+A_1\frac{h^4}{360}u^6(x)+\cdots \\
&+A_2u^2(x)+A_2\frac{h^2}{3}u^4(x)+A_2\frac{2h^4}{45}u^6(x)+\cdots \\
&= u^2(x)\left(A_1+A_2\right)+h^2u^4(x)\left(\frac{A_1}{12}+\frac{A_2}{3}\right) \\
&\qquad +h^4u(x)\left(\frac{A_1}{360}+\frac{2A_2}{45}\right)+\cdots
\end{aligned}$$

or

$$= u''(x)\left(A_1+A_2\right)+h^2u^4(x)\left(\frac{A_1}{12}+\frac{A_2}{3}\right)+O(h^4). \tag{1.16}$$

As our target is to obtain fourth order central finite difference approximation, so we must have

$$A_1+A_2=1 \quad \text{and} \quad A_1+4A_2=0.$$

Solving simultaneously these two equations, we have

$$A_1=\frac{4}{3} \quad \text{and} \quad A_2=-\frac{1}{3}.$$

By substituting the values of A_1 and A_2 in equation (1.16) , we get the required *fourth order central finite difference approximation of* $u''(x)$, given by

$$u''(x)\approx\frac{4}{3}\left[\frac{u(x+h)-2u(x)+u(x-h)}{h^2}\right]-\frac{1}{3}\left[\frac{u(x+2h)-2u(x)+u(x-2h)}{4h^2}\right]$$

or

$$u''(x)\approx\frac{1}{12h^2}\left[-u(x+2h)+16u(x+h)-30u(x)+16u(x-h)-u(x-2h)\right]. \tag{1.17}$$

Which is widely known form in the literature [11, 16].

1.11.3 Sixth order central finite difference approximation

Following the same procedure used above, we introduce two more nodes to the previously existing four nodes, that are $(x+3h)$ and $(x-3h)$, and their corresponding Taylor's series approximations are.

$$u(x+3h) = u(x) + 3hu'(x) + \frac{9h^2}{2!}u''(x) + \frac{27h^3}{3!}u'''(x) + \frac{81h^4}{4!}u^4(x)$$
$$+\frac{243h^5}{5!}u^5(x) + \frac{729h^6}{6!}u^6(x) + \frac{2187h^7}{7!}u^7(x) + \frac{6561h^8}{8!}u^8(x) + \cdots$$

and

$$u(x-3h) = u(x) - 3hu'(x) + \frac{9h^2}{2!}u''(x) - \frac{27h^3}{3!}u'''(x) + \frac{81h^4}{4!}u^4(x)$$
$$-\frac{243h^5}{5!}u^5(x) + \frac{729h^6}{6!}u^6(x) - \frac{2187h^7}{7!}u^7(x) + \frac{6561h^8}{8!}u^8(x) - \cdots$$

adding the above two equations, we get

$$u(x+3h)+u(x-3h) = 2u(x)+9h^2u^2+\frac{27}{4}h^4u^4(x)+\frac{81}{40}h^6u^6(x)+\frac{729}{2240}h^8u^8(x)+\cdots$$

or

$$\frac{u(x+3h) - 2u(x) + u(x-3h)}{9h^2} = u^2+\frac{3}{4}h^2u^4(x)+\frac{9}{40}h^4u^6(x)+\frac{81}{2240}h^6u^8(x)+\cdots .$$

Next, keeping in mind our aim, we have to consider the linear combination of the following three equations.

$$\left[\frac{u(x+h) - 2u(x) + u(x-h)}{h^2}\right] = u''(x) + \frac{h^2}{12}u^4(x) + \frac{h^4}{360}u^6(x) + \cdots \quad (1.18)$$

$$\left[\frac{u(x+2h) - 2u(x) + u(x-2h)}{4h^2}\right] = u''(x) + \frac{1}{3}h^2u^4(x) + \frac{2}{45}h^4u^6(x) + \cdots \quad (1.19)$$

and

$$\left[\frac{u(x+3h) - 2u(x) + u(x-3h)}{9h^2}\right] = u''(x)+\frac{3}{4}h^2u^4(x)+\frac{9}{40}h^4u^6(x)+\frac{81}{2240}h^6u^8(x)+\cdots \quad (1.20)$$

To write a linear combination, multiplying equation (1.18), (1.19), and (1.20) by A_1, A_2 and A_3 respectively, afterwards adding them, we have

$$
\begin{aligned}
&A_1\left[\frac{u(x+h)+u(x-h)-2u(x)}{h^2}\right]+A_2\left[\frac{u(x+2h)+u(x-2h)-2u(x)}{4h^2}\right]+\\
&A_3\left[\frac{u(x+3h)-2u(x)+u(x-3h)}{9h^2}\right]=A_1u^2(x)+A_1\frac{h^2}{12}u^4+A_1\frac{h^4}{360}u^6\\
&A_1\frac{h^6}{20160}u^8(x)+A_2u^2+A_2\frac{h^2}{3}u^4+A_2\frac{2h^4}{45}u^6+\\
&A_2\frac{4h^6}{315}u^8(x)+A_3u^2+A_3\frac{3h^2}{4}u^4+A_3\frac{9h^4}{40}u^6+\\
&A_3\frac{81h^6}{2240}u^8(x)+\cdots\\
&=(A_1+A_2+A_3)u^2(x)+h^2\left(\frac{A_1}{12}+\frac{A_2}{3}+\frac{3A_3}{4}\right)u^4(x)+\\
&h^4\left(\frac{A_1}{360}+\frac{2A_2}{45}+\frac{9A_3}{40}\right)u^6(x)+h^6\left(\frac{A_1}{20160}+\frac{4A_2}{315}+\frac{81A_3}{2240}\right)u^8+\cdots.\\
&=(A_1+A_2+A_3)u^2(x)+h^2\left(\frac{A_1}{12}+\frac{A_2}{3}+\frac{3A_3}{4}\right)u^4(x)+\\
&h^4\left(\frac{A_1}{360}+\frac{2A_2}{45}+\frac{A_3}{40}\right)u^6(x)+O(h^6).
\end{aligned}
\tag{1.21}
$$

Therefore, in order to get *sixth* order accuracy, we must have

$$A_1+A_2+A_3=1,$$

$$A_1+4A_2+9A_3=0,$$

$$\text{and} \qquad A_1+16A_2+81A_3=0.$$

Solving the above three equations simultaneously, we get the following values.

$$A_1=\frac{3}{2}, \qquad A_2=-\frac{3}{5}, \qquad \text{and } A_3=\frac{1}{10}.$$

Substituting the values of these $A_i's$, $i=1,2,3$ back in equation (1.21), and after simplification we get the *sixth order central finite difference approximation of* $u''(x)$, i.e;

$$u''(x)\approx\frac{3}{2}\left[\frac{u(x+h)-2u(x)+u(x-h)}{h^2}\right]-\frac{3}{5}\left[\frac{u(x+2h)-2u(x)+u(x-2h)}{4h^2}\right]$$

$$+\frac{1}{10}\left[\frac{u(x+3h)-2u(x)+u(x-3h)}{9h^2}\right]$$

or

$$\begin{aligned} u''(x) \approx \frac{1}{180h^2}&[2u(x+3h)-27u(x+2h)+270u(x+h)-490u(x)\\ &+270u(x-h)-27u(x-2h)+2u(x-3h). \end{aligned} \tag{1.22}$$

It is widely known form in the literature [11, 16].

Now, in general, the number of equations involving unknowns, which define the order of approximation of second order derivative, can be written as [16],

$$A_1 + A_2 + \cdots + A_{k+1} = 1,$$

$$\begin{aligned} A_1 + 2^2 A_2 + \cdots + (k+1)^2 A_{k+1} &= 0,\\ A_1 + 2^4 A_2 + \cdots + (k+1)^4 A_{k+1} &= 0,\\ \vdots \qquad \vdots \qquad\qquad \vdots &= \quad \vdots,\\ A_1 + 2^{2k} A_2 + \cdots + (k+1)^{2k} A_{k+1} &= 0. \end{aligned}$$

Whereas, the compact form for finding these $A_j's$, $j = 1, 2, \cdots, k+1$ is defined as,

$$A_j = \prod_{l=1, l\neq j}^{k+1} \frac{l^2}{l^2 - j^2}$$

where $j = 1, 2, 3, \ldots, k+1$. The coefficients of $A_j's$ make the Vandormonde Matrix.

The values of these $A_j's$ depending upon the order of approximation of $u''(x)$, can be put in a tabular form [16], as follows in Table 1.2.

Note that the number of $A_j's$ involved are equal to half the order of the central finite difference approximation of second order derivative.

1.12 Central finite difference schemes for Helmholtz equation

As the central topic of this thesis is the construction of dispersion free central finite difference schemes for the wave equation, which involves second order partial

Order	A_1	A_2	A_3	A_4	A_5	A_6	A_7
$O(h^2)$	1						
$O(h^4)$	$\frac{4}{3}$	$-\frac{1}{3}$					
$O(h^6)$	$\frac{3}{2}$	$-\frac{3}{5}$	$\frac{1}{10}$				
$O(h^8)$	$\frac{8}{5}$	$-\frac{4}{5}$	$\frac{8}{35}$	$-\frac{1}{35}$			
$O(h^{10})$	$\frac{5}{3}$	$-\frac{20}{21}$	$\frac{5}{14}$	$-\frac{5}{63}$	$\frac{1}{126}$		
$O(h^{12})$	$\frac{12}{7}$	$-\frac{15}{14}$	$\frac{10}{21}$	$-\frac{1}{7}$	$\frac{2}{77}$	$-\frac{1}{462}$	
$O(h^{14})$	$\frac{7}{4}$	$-\frac{7}{6}$	$\frac{7}{12}$	$-\frac{7}{33}$	$\frac{7}{132}$	$-\frac{7}{858}$	$\frac{1}{1716}$

Table 1.2: Table of central finite difference coefficients

derivatives with respect to both space and time. Whereas, in the beginning for the sake of simplicity and understanding, we will construct second, fourth and sixth order central finite difference schemes for the Helmholtz equation, which contains only spatial second order derivative, that makes it easier to study. Then, we will measure the difference $\tilde{k} - k$ for these central finite difference schemes. It will give us an insight about the quantitative as well as the qualitative behavior of dispersion inherited by these schemes [1, 2, 16, 35, 40].

1.12.1 Second order central finite difference scheme

Reconsider the one dimensional Helmholtz equation (1.8), derived in the initial section

$$u''(x) + k^2 u(x) = 0.$$

Now replacing $u''(x)$ with its standard second order central finite difference approximation, defined in (1.13), we have

$$\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + k^2 u(x) = 0$$

rearranging above, gives us the following scheme.

$$u(x+h) - (2 - h^2 k^2) u(x) + u(x-h) = 0. \tag{1.23}$$

This is the standard 3−point, second order, central finite difference scheme for Helmholtz equation with step length, h.

1.12.2 Dispersion relation for second order central finite difference scheme

Let us calculate the dispersion in (1.23) scheme. For this, we use the plane wave solution (1.9), of the following form

$$u(x) \;=\; Ae^{i\tilde{k}x} + Be^{-i\tilde{k}x}, \qquad \text{where } \tilde{k} = \text{discrete wave number}. \tag{1.24}$$

Whereas,

$$\begin{aligned} u(x+h) &= Ae^{i\tilde{k}(x+h)} + Be^{-i\tilde{k}(x+h)} \\ u(x-h) &= Ae^{i\tilde{k}(x-h)} + Be^{-i\tilde{k}(x-h)}. \end{aligned}$$

Here, $\tilde{k}$ is used instead of k. Because, we are intrusted in writing the dispersion relation and the difference of discrete wave number and continues wave number gives the required expression.

Substituting the values of $u(x+h)$, u(x), $u(x-h)$ in (1.23), and simplifying we have the form,

$$(2\cos(\tilde{k}h) - 2 + h^2k^2)u(x) = 0.$$

since, $2\cos(\tilde{k}h) = e^{i\tilde{k}h} + e^{-i\tilde{k}h}$.

For a non trivial solution we have $u(x) \neq 0$, so

$$2\cos(\tilde{k}h) - 2 + h^2k^2 = 0.$$

We solve the above expression for $\tilde{k}h$,

$$\begin{aligned} \cos(\tilde{k}h) &= 1 - \frac{1}{2}h^2k^2 \\ \tilde{k}h &= \cos^{-1}\left(1 - \frac{1}{2}h^2k^2\right). \end{aligned}$$

After the simplification, we have the next relation

$$\tilde{k} - k = \frac{1}{24}k^3h^2 + \cdots. \tag{1.25}$$

or we can write it as follows,

$$\frac{\tilde{k}}{k} - 1 = \frac{1}{24}(kh)^2 + \cdots.$$

As $k = (\omega/c)$ and $\tilde{k} = (\omega/\tilde{c})$, using these relations in (1.25), we get

$$\frac{\omega}{\tilde{c}} - \frac{\omega}{c} = \frac{1}{24}\left(\frac{\omega}{c}\right)^3 h^2 + \cdots.$$

Rearranging and simplifying the above expression, we have

$$\frac{c}{\tilde{c}} - 1 = \frac{1}{24}\left(\frac{\omega h}{c}\right)^2 + \cdots.$$

This is the required alternative approach to observe the dispersion. From the expression (1.25) one can clearly see that $\tilde{k} - k \neq 0$, it means that dispersion is present in the second order central finite difference scheme and the following observations can be made;
(a) Here the coefficient of the leading term is (1/24), and that it is (1/2) times the coefficient of the leading term in a second order central finite difference approximation of $u''(x)$; (b) The positive sign in this dispersion relation shows the lag of the numerical wave by using second order central finite difference scheme, in comparison with that of the exact wave; (c) If $k^3h^2 \to 0$ in (1.25) then $\frac{\tilde{k}}{k} = 1$, which requires very very fine mesh, even for a moderate value of the wavenumber, k. So, the best option is to go for higher order schemes.

1.12.3 Fourth order central finite difference scheme

Again consider the Helmholtz equation (1.8) and by using the fourth order central finite approximation of $u''(x)$ given in (1.17), we have

$$\frac{1}{12h^2}\left[-u(x+2h) + 16u(x+h) - 30u(x) + 16u(x-h) - u(x-2h)\right] + k^2u(x) = 0$$

which gives the following scheme,

$$16u(x-h) - 32u(x) + 16u(x+h) - u(x-2h) + 2u(x) - u(x+2h) + 12h^2k^2u(x) = 0$$

$$\text{or} \quad 16u(x+h) - u(x+2h) - 6(5-2h^2k^2)u(x) - u(x-2h) + 16u(x-h) = 0. \quad (1.26)$$

This is the required 5-point, fourth order, central finite difference scheme for Helmholtz equation having mesh size, h.

1.12.4 Dispersion relation for fourth order central finite difference scheme

Next, we will talk about its dispersion. Again consider the plane wave solution of the form we used in (1.24), and define the following from it.

$$\begin{aligned}
u(x+h) &= Ae^{i\tilde{k}(x+h)} + Be^{-i\tilde{k}(x+h)} \\
u(x-h) &= Ae^{i\tilde{k}(x-h)} + Be^{-i\tilde{k}(x-h)} \\
u(x+2h) &= Ae^{i\tilde{k}(x+2h)} + Be^{-i\tilde{k}(x+2h)} \\
u(x-2h) &= Ae^{i\tilde{k}(x-2h)} + Be^{-i\tilde{k}(x-2h)}.
\end{aligned}$$

Substitute the values in the equation (1.26), and simplifying we get,

$$\left[\frac{8}{3}(\cos(\tilde{k}h)-1) - \frac{1}{6}(\cos(2\tilde{k}h)-1) + h^2k^2\right] u(x) = 0.$$

Above, we have used these two equalities; $2\cos(\tilde{k}h) = e^{i\tilde{k}h} + e^{-i\tilde{k}h}$ and $2\cos(2\tilde{k}h) = e^{2i\tilde{k}h} + e^{-2i\tilde{k}h}$. For a non trivial solution $u(x) \neq 0$, this implies that

$$\begin{aligned}
\frac{8}{3}(\cos(\tilde{k}h)-1) - \frac{1}{6}(\cos(2\tilde{k}h)-1) + h^2k^2 &= 0 \\
16\cos(\tilde{k}h)-1) - (\cos(2\tilde{k}h)-1) + 6h^2k^2 &= 0 \\
16\cos(\tilde{k}h) - 16 - \cos(2\tilde{k}h) + 1 + 6h^2k^2 &= 0 \\
16\cos(\tilde{k}h) - 15 - \cos(2\tilde{k}h) + 6h^2k^2 &= 0 \\
6h^2k^2 - 15 &= \cos(2\tilde{k}h) - 16\cos(\tilde{k}h) \\
6h^2k^2 - 15 &= 2\cos^2(\tilde{k}h) - 1 - 16\cos(\tilde{k}h) \\
\text{or} \quad 3h^2k^2 + 8 &= (\cos(\tilde{k}h) - 2)^2.
\end{aligned}$$

Further simplify it, we get

$$\tilde{k} - k = \frac{1}{180}k^5h^4 + \cdots . \tag{1.27}$$

it can also be written as,

$$\frac{\tilde{k}}{k} - 1 = \frac{1}{180}(kh)^4 + \cdots .$$

Again, by using the same relation; $k = (\omega/c)$ and $\tilde{k} = (\omega/\tilde{c})$, using them in the (1.27), we get

$$\frac{\omega}{\tilde{c}} - \frac{\omega}{c} = \frac{1}{180}\left(\frac{\omega}{c}\right)^5 h^4 + \cdots .$$

Rearranging and simplifying the above expression, we have

$$\frac{c}{\tilde{c}} - 1 = \frac{1}{180}\left(\frac{\omega h}{c}\right)^4 + \cdots .$$

This is the required alternative approach to observe the dispersion. From the last equation it is clear that dispersion is non zero, also the following observations are made;
(a) The coefficient of the leading term that is 1/180, it is (1/2) times the coefficient of leading term in fourth order central finite difference approximation of $u''(x)$; (b) The positive sign shows the lag of numerical wave by using the fourth order central finite difference scheme when compared with the exact wave; (c) If $k^5h^4 \rightarrow 0$ in (1.27) then we can observe that $\frac{\tilde{k}}{k} = 1$, which requires very fine mesh, even for a moderate value of the wavenumber, k. Whereas, the best option is to go for higher order schemes.

1.12.5 Analysis about mesh size

Here, we have used an interesting approach, we define the value for h_1, which is taken as the step length used in second order C.F.D scheme, in terms of h_2, which is the step length taken in fourth order C.F.D scheme, by considering both the schemes dispersion leading terms equal. The reason of this thought is that, by using this h_1 in the second order C.F.D scheme, gives us fourth order accuracy instead of second order accuracy, but this is very very costly. Thus, to derive the expression consider the error term of standard second order central finite difference scheme, we just calculated in the last section, that is;

$$\tilde{k} - k = \frac{1}{24}k^3h_1^2$$

Scheme	$\tilde{k} - k$	h	$N = \frac{b-a}{h}$
second order C.F.D	$9.97 * 10^{-4}$	0.004891	205
fourth order C.F.D	$9.97 * 10^{-4}$	0.0366	27

Table 1.3: Mesh size comparison of second and fourth order C.F.D schemes with same dispersion error, $\tilde{k} - k$.

and at the same time consider the error term of standard fourth order central finite difference scheme, that is,

$$\tilde{k} - k = \frac{1}{180} k^5 h_2^4.$$

Since, we are intrusted in finding the expression for h_1 such that both the error terms of second and fourth order C.F.D schemes are same, so take

$$\begin{aligned} \frac{1}{24} k^3 h_1^2 &= \frac{1}{180} k^5 h_2^4 \\ \frac{1}{24} h_1^2 &= \frac{1}{180} k^3 h_2^4 \\ h_1^2 &= \frac{2}{15} k^2 h_2^4 \end{aligned}$$

$$\text{or} \quad h_1 = \sqrt{\frac{2}{15}} k h_2^2. \tag{1.28}$$

Hence, by using this h_1 in second order C.F.D scheme, we will get accuracy level of fourth order C.F.D scheme.

In order to have a clear understanding of this new concept, the Table 1.3 is constructed. To make the table, it is said that we require fourth order accuracy by using three point standard central finite difference scheme of Helmholtz equation, with given $h_2 = 0.0366$ and $k = 10$, where $0 \leq x \leq 1$. We have used the relation (1.25) and (1.27) to get the value of $\tilde{k} - k$ in the table, and (1.28) to get the value of h_1.

From the Table 1.3 it is clear that, if we use the second order scheme with h_1 calculated from (1.28) we get 10^{-4} accuracy as well as we need 205 number of elements, it is comparatively very high if we get the same accuracy by using the fourth order scheme with h_2, and only 27 elements. Hence, the higher order schemes are relatively cheaper to use.

1.12.6 Sixth order central finite difference scheme

This time we take the sixth order approximation of $u''(x)$ defined in equation (1.22), involved in Helmholtz equation.

$$\frac{1}{180h^2}[2u(x+3h)-27u(x+2h)+270u(x+h)-490u(x)+270u(x-h)-27u(x-2h)+2u(x-3h)]$$
$$+k^2u(x)=0.$$

After simplification we have,

$$270(u(x-h)-2u(x)+270u(x+h))-27(u(x-2h)-2u(x)+u(x+2h))$$
$$+2(u(x-3h)-2u(x)+u(x+3h))+180h^2k^2u(x)=0$$

or, we can write it as

$$2u(x+3h)-27u(x+2h)+270u(x+h)-10(49-18h^2k^2)u(x)$$
$$+270u(x-h)-27u(x-2h)+2u(x-3h)=0. \quad (1.29)$$

This is the required 7−point, sixth order central finite difference scheme for Helmholtz equation.

1.12.7 Dispersion relation for sixth order central finite difference scheme

In order to compute the dispersion relation, consider the exact solution (1.24), of Helmholtz equation of the following form,

$$u(x)=A^{i\tilde{k}x}+Be^{-i\tilde{k}x}$$

then, we can define the following

$$\begin{aligned}
u(x+h) &= Ae^{i\tilde{k}(x+h)} + Be^{-i\tilde{k}(x+h)} \\
u(x-h) &= Ae^{i\tilde{k}(x-h)} + Be^{-i\tilde{k}(x-h)} \\
u(x+2h) &= Ae^{i\tilde{k}(x+2h)} + Be^{-i\tilde{k}(x+2h)} \\
u(x-2h) &= Ae^{i\tilde{k}(x-2h)} + Be^{-i\tilde{k}(x-2h)} \\
u(x+3h) &= Ae^{i\tilde{k}(x+3h)} + Be^{-i\tilde{k}(x+3h)} \\
u(x-3h) &= Ae^{i\tilde{k}(x-3h)} + Be^{-i\tilde{k}(x-3h)}.
\end{aligned}$$

Using these substitutions in (1.29) and then simplify, we get,

$$[3\cos(\tilde{k}h) - 1) - \frac{3}{10}(\cos(2\tilde{k}h) - 1) + \frac{1}{45}(\cos(3\tilde{k}h) - 1) + h^2k^2]u(x) = 0$$

since, we know that $2\cos(\tilde{k}h) = e^{i\tilde{k}h} + e^{-i\tilde{k}h}$, $2\cos(2\tilde{k}h) = e^{2i\tilde{k}h} + e^{-2i\tilde{k}h}$ and $2\cos(3\tilde{k}h) = e^{3i\tilde{k}h} + e^{-3i\tilde{k}h}$. For a nontrivial solution $u(x) \neq 0$, so

$$3(\cos(\tilde{k}h) - 1) - \frac{3}{10}(\cos(2\tilde{k}h) - 1) + \frac{1}{45}(\cos(3\tilde{k}h) - 1) + h^2k^2 = 0$$

$$h^2k^2 = -3(\cos(\tilde{k}h) - 1) + \frac{3}{10}(\cos(2\tilde{k}h) - 1) - \frac{1}{45}(\cos(3\tilde{k}h) - 1)$$

further simplification gives us,

$$\tilde{k} - k = \frac{1}{1120}k^7h^6 + \cdots . \tag{1.30}$$

$$\frac{\tilde{k}}{k} - 1 = \frac{1}{1120}(kh)^6 + \cdots .$$

Again, by using the relations; $k = (\omega/c)$ and $\tilde{k} = (\omega/\tilde{c})$, in the above defined $\tilde{k} - k$, we get

$$\frac{\omega}{\tilde{c}} - \frac{\omega}{c} = \frac{1}{1120}\left(\frac{\omega}{c}\right)^7 h^6 + \cdots .$$

Rearranging and simplifying the above expression, we have

$$\frac{c}{\tilde{c}} - 1 = \frac{1}{1120}\left(\frac{\omega h}{c}\right)^6 + \cdots .$$

It is the required alternative approach for dispersion. From (1.30) we can see the dispersion is non zero, and the following observations are made;

(a) The coefficient of the leading which is (1/1120), it is (1/2) times the order of the leading term coefficient of sixth order central finite difference approximation of $u''(x)$; (b) The positive sign shows the lag of the numerical wave by using sixth order finite difference scheme when compared with the exact wave; (c) If $k^7h^6 \to 0$ in (1.30) then it gives $\dfrac{\tilde{k}}{k} = 1$, which requires a little fine mesh comparatively to fourth and second order schemes.

1.12.8 Analysis about mesh size

Here again we have made the same observation, and calculated the value of h_1, step length of second order C.F.D scheme in terms of h_3, which is the step length of sixth order C.F.D scheme. So, consider the error terms of the second and sixth order standard central finite difference schemes, which are given below respectively.

$$\tilde{k} - k = \frac{1}{24}k^3h_1^2.$$

and

$$\tilde{k} - k = \frac{1}{1120}k^7h_3^6.$$

Similarly, we can find the expression for h_1, by taking both the error terms same.

$$\begin{aligned} \frac{1}{24}k^3h_1^2 &= \frac{1}{1120}k^7h_3^6 \\ h_1^2 &= \frac{3}{140}k^4h_3^6. \end{aligned}$$

$$\text{or} \qquad h_1 = \sqrt{\frac{3}{140}}k^2h_3^3. \tag{1.31}$$

Hence, by using the above h_1, in our second order C.F.D scheme we will obtain the sixth order accuracy.

1.12.9 Analysis about mesh size

In this part, we have derived the expression for h_2, that is the step length in fourth order C.F.D scheme, in terms of h_3, which is the step length of sixth order C.F.D scheme. We will follow the same procedure, consider the error terms of the fourth and sixth order standard central finite difference schemes, that are given below respectively.

$$\tilde{k} - k = \frac{1}{180} k^5 h_2^4$$

and

$$\tilde{k} - k = \frac{1}{1120} k^7 h_3^6$$

we have to find the expression for h_2, in which both the error terms are taken to be the same. So,

$$\begin{aligned} \frac{1}{180} k^5 h_2^4 &= \frac{1}{1120} k^7 h_3^6 \\ h_2^4 &= \frac{9}{56} k^2 h_3^6 \end{aligned}$$

$$\text{or} \quad h_2 = \sqrt[4]{\frac{9}{56} k^2 h_3^6}. \tag{1.32}$$

Consequently, using the above h_2 in the fourth order C.F.D scheme, will give us the sixth order accuracy. Similarly, the following Table 1.4 is constructed, in which it is said that we require the sixth order accuracy at first by using the three point C.F.D scheme for Helmholtz equation and then secondly by using the five point C.F.D scheme for Helmholtz equation, with given $h_3 = 0.05$ and $k = 10$, $0 \leq x \leq 1$. We have used the relations (1.25), (1.27) and (1.30), in order to get the value of $\tilde{k} - k$ in the table. Whereas, to calculate the values of h_1 and h_2 we have used (1.31) and (1.32) respectively.

From the Table 1.4, one can easily comprehend that the higher order schemes are inexpensive and require less labor, which makes them more desirable to use. In the next Table 1.5, we have used (1.25), (1.27) and (1.30), such that $\tilde{k}-k = 10^{-3}$ and $k = 15$, where $0 \leq x \leq 1$. In order to observe the advantage of higher order schemes, in the standard and very simple manner.

Another Table 1.6 is added, in order to analyze the effects of a given wave number k, on mesh size h and then on number of elements N, such that we require

Scheme	$\tilde{k}-k$	h	N
Second order C.F.D	$1.4 * 10^{-4}$	0.001830	546
Fourth order C.F.D	$1.39 * 10^{-4}$	0.022380	44
sixth order C.F.D	$1.4 * 10^{-4}$	0.05	20

Table 1.4: Mesh size comparison of second, fourth, and sixth order schemes with same dispersion error, $\tilde{k}-k$.

Scheme order	h	$N = \frac{b-a}{h}$
second	0.002667	375
Fourth	0.022065	45
Sixth	0.043261	23

Table 1.5: Comparison of schemes.

$\tilde{k} - k > 10^{-4}$, where $0 \leq x \leq 1$.

From the Table 1.6 it is clear that, while reading the table vertically we can observe that as the wave number increases the value of h decreases, consequently increasing the number of elements. It means that with a large value of k we have to use very very small mesh, to get the required accuracy. Whereas, the second aspect of the table is visible when we read it horizontally in which we can see the values

wave number	$2nd$ order scheme	$4th$ order scheme	$6th$ order scheme
k	(h,N)appx	(h,N)appx	(h,N)appx
10	(0.001549,646)	(0.020598,49)	(0.047301,21)
20	(0.000548,1825)	(0.008660,115)	(0.021070,47)
30	(0.000298,3356)	(0.005217,192)	(0.013129,76)
40	(0.000194,5155)	(0.003641,275)	(0.009386,107)

Table 1.6: Analysis about wave number.

Mesh size	Nodes	$2nd$ order scheme	$4th$ order scheme	$6th$ order scheme
h	N	$\tilde{k} - k$	$\tilde{k} - k$	$\tilde{k} - k$
0.001	1000	$1.40625 * 10^{-4}$	$4.21875 * 10^{-9}$	$1.525530134 * 10^{-13}$
0.0025	400	$8.7890625 * 10^{-4}$	$1.647949219 * 10^{-7}$	$3.724438804 * 10^{-11}$
0.005	200	$3.515625 * 10^{-3}$	$2.63671875 * 10^{-6}$	$2.383595844 * 10^{-10}$
0.0075	133	$7.91015625 * 10^{-3}$	$1.334838867 * 10^{-5}$	$2.715064641 * 10^{-9}$
0.01	100	0.0140625	$4.21875 * 10^{-5}$	$1.52550134 * 10^{-8}$
0.025	40	0.087890625	$1.647949219 * 10^{-3}$	$3.724368506 * 10^{-6}$
0.05	20	0.3515625	0.0263671875	$2.383595844 * 10^{-4}$
0.075	13	0.791015625	0.1334838867	$2.715064641 * 10^{-3}$

Table 1.7: Analysis about the order of accuracy in different schemes.

of h and N in second, fourth and sixth order schemes for Helmholtz equation. If we observe this side of the table, it is evident that with an increase in the order of scheme, on the contrary to above the value of h increases consequently, decreasing the number of elements. Indicating that higher order schemes are preferred as they are time saving.
Similarly, in order to analyze the effect of a given mesh size h, with $k = 15$ fixed, on number of elements N and on the order of $\tilde{k} - k$, with second, fourth and sixth order central finite difference schemes for Helmholtz equation, the next Table 1.7 is constructed.

While reading the Table 1.7 vertically it is clear that, when h increases then the no of elements decreases, which reduces the computational cost but at the same time it decreases the order of accuracy. If we read the table horizontally, where the order of the scheme increases, we can observe that the order of accuracy improves.

1.13 Reducing the phase error for finite difference method without increasing the order, [1]

Here, we will review the idea presented by Nehrbas and Lee [1]. They found a dispersion controlling parameter α for the second order central finite difference scheme for Helmholtz equation. By making a simple modification in the standard second order central finite difference scheme, that is, replacing the central node weight 2 by α. Further, showing that when α is used in second order central finite difference scheme instead of 2, the novel scheme is numerically dispersion free.
The following problem was solved in [1]:

$$u''(x) + k^2 u(x) = 0, \quad x \in (0, 1)$$

with boundary conditions as,

$$u(0) = 1, \quad \text{and} \quad u'(1) - iku(1) = 0.$$

The approximation defined for second order derivative is,

$$u''(x) \approx \frac{u(x+h) - \alpha u(x) + u(x-h)}{h^2}.$$

By using the above defined $u''(x)$ approximation in Helmholtz equation and after simplification, we are left with the following scheme.

$$u(x+h) - (\alpha - h^2k^2)u(x) + u(x-h) = 0. \tag{1.33}$$

This involves an unknown α. In the next step, the value of α is calculated, and to do so, we need the aid of an exact solution. Consider a plane wave solution of the form

$$u(x) = Ae^{ikx} + Be^{-ikx}.$$

We get

$$\begin{aligned} u(x+h) &= Ae^{ik(x+h)} + Be^{-ik(x+h)}, \\ u(x-h) &= Ae^{ik(x-h)} + Be^{-ik(x-h)}. \end{aligned}$$

Substituting the values of $u(x+h)$, $u(x-h)$ and u(x) defined above in (1.33), and after simplification we are left with the following,

$$(2\cos(kh) - \alpha + h^2k^2)u(x) = 0$$

For a non trivial solution $u(x) \neq 0$. So,

$$2\cos(kh) - \alpha + h^2k^2 = 0,$$

which gives

$$\alpha = h^2k^2 + 2\cos(kh).$$

Replacing α by its value in equation (1.33). We get the following novel scheme for the Helmholtz equation.

$$u(x-h) - 2\cos(kh)u(x) + u(x+h) = 0. \tag{1.34}$$

As it was said earlier that, this novel scheme is numerically dispersion less. So, one can see that by calculating the dispersion relation for scheme (1.34). For this purpose set

$$u(x) = Ae^{i\tilde{k}x} + Be^{-i\tilde{k}x},$$

and further;

$$\begin{aligned} u(x+h) &= Ae^{i\tilde{k}(x+h)} + Be^{-i\tilde{k}(x+h)}, \\ u(x-h) &= Ae^{i\tilde{k}(x-h)} + Be^{-i\tilde{k}(x-h)}. \end{aligned}$$

Inserting the values in the scheme (1.34), and simplifying we get.

$$(2\cos(\tilde{k}h) - 2\cos(kh))u(x) = 0.$$

For a non trivial solution $u(x) \neq 0$, thus

$$\cos(\tilde{k}h) - \cos(kh) = 0$$

the last expression gives,

$\tilde{k} - k = 0$, meaning that there is no numerical dispersion in (1.34), and hence it proves the claim.

We have proposed the following system to solve the above defined one dimensional problem following [1]:

$$\begin{aligned} u(x) &= 1, \\ \text{at } \ x = 0 & \\ u(x+h) - 2\cos(hk)u(x) + u(x-h) &= 0, \\ \text{at } \ x = 1, 2, \ldots (N-1) & \\ (ihk - \cos(hk))u(x) + u(x-h) &= 0. \\ \text{at } \ x = N & \end{aligned}$$

The following are the traits which we have comprehended from this paper: (a) its a simple idea; (b) gives exact interior points; (c) numerically dispersion less scheme in one dimension; (d) no need to write a new code, altogether; (e) it is a general form, we can go back to standard one, but; (f) it is not good for high wave number, and; (g) one need to know the exact solution before hand.

1.14 Summary of results

So far, from the analysis of paper [1], we have composed the results in a tabular form. See Table 1.8 for a quick review of paper [1].

1.15 Observations of one and two dimensional schemes:

In Table 1.9, we have summarized the results of one and two dimensional novel second order schemes for Helmholtz equation, presented in paper [1].

Second order C.F.D.S	Central node, α	dispersion term, $(\tilde{k}-k)$
standard	2	$\frac{1}{24}k^3h^2$
novel	$h^2k^2+2\cos(kh)$	0
improved	$2+\frac{1}{12}h^4k^4$	$-\frac{1}{720}k^5h^4$

Table 1.8: Second order C.F.D schemes.

Name	In one dimension	In two dimension (square mesh)
Problem equation	$u''(x) + k^2 = 0$	$u_{xx} + u_{yy} + k^2 u(x,y) = 0$
Plane wave solution	$u(x) = e^{ikx}$	u(x,y)=$e^{ik(x\cos\theta + y\sin\theta)}$
Time harmonic substitution	u(x,t)=u(x)$e^{i\omega t}$	u(x,y,t)=u(x,y)$e^{i\omega t}$
Standard second order C.F.D.S	$u(x+h) - (2 - h^2k^2)u(x) + u(x-h) = 0$	$u(x+h,y) + u(x,y+h) - (4 - h^2k^2)u(x,y)$ $+u(x,y-h) + u(x-h,y) = 0$
Dispersion	$\tilde{k} - k = \frac{1}{24}k^3h^2$	$\tilde{k} - k = \frac{1}{24}(\sin^3\theta + \cos^3\theta)k^3h^2$
Novel scheme	$u(x+h) - (\alpha - h^2k^2)u(x) + u(x-h) = 0$	$u(x+h,y) + u(x,y+h) - (2\alpha - h^2k^2)u(x,y)$ $+u(x,y-h) + u(x-h,y) = 0$
Value of α	$\alpha = 2\cos(kh) + h^2k^2$	$\alpha = \frac{1}{2}h^2k^2 + \cos(k_1h) + \cos(k_2h)$

Table 1.9: One and two dimensional novel schemes.

1.16 Exact finite difference schemes for solving Helmholtz equation at any wavenumber, [2]

In this section, we will review the idea given by Yau Shu and Li, presented in [2]. One can say that to some extent, it is an extension of the idea of [1], but with a different approach. Since, there was still room for improvement in the proposed idea of [1]. Yau Shu and Li did not only made the finite difference scheme exact but also made the non−reflecting boundary condition exact, since it also involves the first order derivative, and this concept gives us optimal results. With this amendment we get the exact interior as well as the exact boundary points. Hence, there is no question of numerical dispersion at all, in the new scheme. The very important aspect of this scheme is that it is valid for any wave number, k. Again the same problem is solved in this paper, that is

$$u''(x) + k^2u(x) = 0, \quad x \in (0, 1)$$

with boundary conditions as,

$$u(0) = 1, \quad \text{and} \quad u'(1) - iku(1) = 0.$$

From the Helmholtz equation the recursive relation is developed in the following manner for the even order derivatives. One can write (1.8) as,

$$u''(x) = -k^2u(x).$$

In the similar way,

$$\begin{aligned}
u^4(x) &= k^4u(x) \\
u^6(x) &= -k^6u(x) \\
u^8(x) &= k^8u(x) \\
\vdots &= \vdots \\
u^{2n}(x) &= (-1)^nk^{2n}u(x) \qquad n = 1, 2, 3, \cdots .
\end{aligned}$$

Consider the Taylor's series expansion,

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \frac{h^4}{4!}u^4(x) + \cdots$$

and

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2!}u''(x) - \frac{h^3}{3!}u'''(x) + \frac{h^4}{4!}u^4(x) + \cdots .$$

by adding the above two equations, we get

$$\begin{aligned} u(x+h) + u(x-h) &= 2u(x) + 2\frac{h^2}{2!}u''(x) + 2\frac{h^4}{4!}u^4(x) + \cdots \\ u(x+h) + u(x-h) &= 2\left[u(x) + \frac{h^2}{2!}u''(x) + \frac{h^4}{4!}u^4(x) + \cdots\right]. \end{aligned}$$

Using the iterative relation, substitute the even order derivatives by their values, it gives

$$\begin{aligned} u(x+h) + u(x-h) &= 2\left[u(x) + \frac{h^2}{2!}(-k^2u(x)) + \frac{h^4}{4!}(k^4u(x)) + \cdots\right] \\ u(x+h) + u(x-h) &= 2u(x)\left[1 - \frac{hk^2}{2!} + \frac{hk^4}{4!} - \cdots\right] \\ u(x+h) + u(x-h) &= 2\cos(hk)u(x). \end{aligned}$$

Ultimately using it in the approximation of $u''(x)$, with α as a weight of central node in second order C.F.D approximation of $u''(x)$. Then it will give us the novel scheme, written below.

$$u(x+h) - 2\cos(hk)u(x) + u(x-h) = 0.$$

In the similar way, from the non−reflecting boundary condition the recursive relation for the odd order derivatives are calculated in the following manner,

$$\text{as} \qquad u'(x) = iku(x)$$

further,

$$\begin{aligned}
u^3(x) &= -ik^3u(x) \\
u^5(x) &= ik^5u(x) \\
u^7(x) &= -ik^7u(x) \\
\vdots &= \vdots \\
u^{2n-1}(x) &= (-1)^{n+1}ik^{2n-1}u(x) \;\; n = 1, 2, 3, \cdots .
\end{aligned}$$

Again consider the Taylor's series expansion,

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \frac{h^4}{4!}u^4(x) + \cdots$$

and

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2!}u''(x) - \frac{h^3}{3!}u'''(x) + \frac{h^4}{4!}u^4(x) + \cdots .$$

by subtracting the above two equations, we get

$$\begin{aligned}
u(x+h) - u(x-h) &= 2hu'(x) + 2\frac{h^3}{3!}u'''(x) + 2\frac{h^5}{5!}u^5(x) + \cdots \\
u(x+h) - u(x-h) &= 2\left[hu'(x) + \frac{h^3}{3!}u'''(x) + \frac{h^5}{5!}u^5(x) + \cdots\right].
\end{aligned}$$

Using the iterative relation, substitute the odd order derivatives by their values, it gives

$$\begin{aligned}
u(x+h) - u(x-h) &= 2\left[ihku(x) + \frac{h^3}{3!}(-ik^3u(x)) + \frac{h^5}{5!}(ik^5u(x)) + \cdots\right] \\
u(x+h) - u(x-h) &= 2iu(x)\left[hk - \frac{hk^3}{3!} + \frac{hk^5}{5!} - \cdots\right] \\
u(x+h) - u(x-h) &= 2i\sin(hk)u(x).
\end{aligned}$$

This is the required exact non−reflecting boundary condition. For the idea presented in this paper, we have proposed the following system to solve the above defined one dimensional problem.

$$
\begin{aligned}
u(x) &= 1, \\
\text{at } x = 0 & \\
u(x+h) - 2\cos(hk)u(x) + u(x-h) &= 0, \\
\text{at } x = 1, 2, \ldots (N-1) & \\
(i\sin(hk) - \cos(hk))u(x) + u(x-h) &= 0. \\
\text{at } x = N &
\end{aligned}
$$

We have listed few traits of this novel scheme, which are as follows: (a) its a simple idea; (b) exact interior and boundary points; (c) dispersion less scheme in one dimension; (d) no need to write a new code, altogether; (e) general form, we can go back to standard one; (f) good for low as well as high wave number; (g) do not require fine mesh size, and; (h) before hand one do not need the exact solution. In the Figure 1.8, both the novel schemes waves presented in [1] and [2], have same exact behaviour. Since, in Figure 1.8 the wave number is moderate that is $k = 30$, and no of elements are $N = 20$. Whereas, in the same figure we can clearly see that the standard scheme wave is showing dispersion. In the second Figure 1.9, the superiority of [2] on [1] is clearly visible, as the wave number is increased to 100, with same number of elements that is $N = 20$. Whereas, the standard scheme wave has totally dissipated.

Computational wave propagation is an independent as well as an active area of research. Since, it finds applications in many disciplines of life [1, 2, 3, 7, 8, 9, 16, 17] and [18, 19, 20, 29, 30, 35, 39, 40]. So developing an efficient and an accurate numerical method for solving wave equation, is of vital importance and objective of many. Realizing this mathematicians, engineers and physicist made lots of efforts to develop numerical techniques, based upon the discretisation of the domain, hence resulting into errors like numerical dispersion and numerical dissipation. The remedy suggested to control (decrease) numerical dispersion, was in the form of dispersion relation preserving schemes. However, other schemes

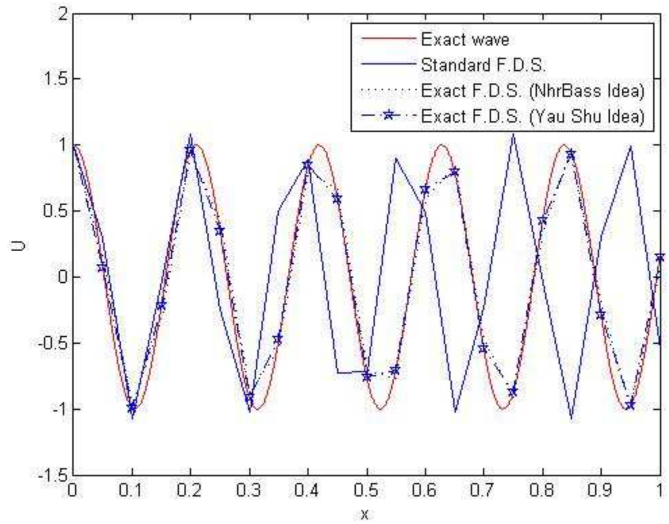

Figure 1.8: $k = 30$, and $N = 20$.

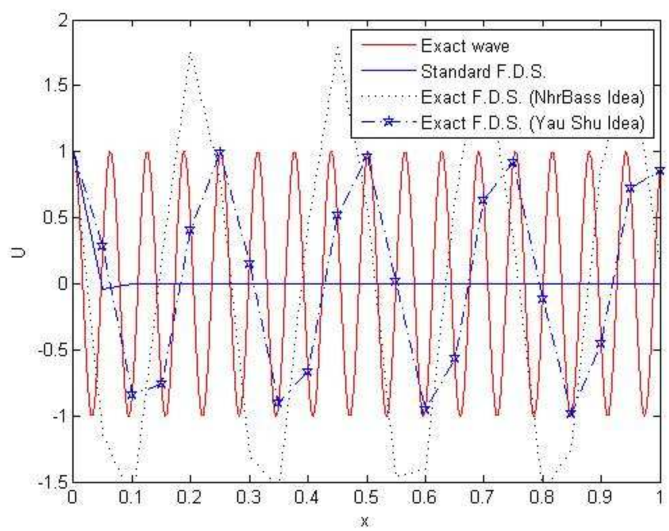

Figure 1.9: $k = 100$, and $N = 20$.

require fine mesh size or higher order schemes, to get the desired level of accuracy [7, 12, 13, 14, 15, 21, 23, 24, 25, 26, 27, 28]. Whereas, one can control numerical dissipation by restricting wave number, k to be real.

Chapter 2
Optimal Finite Difference Schemes For Wave Equation

Chapter 2

Optimal Finite Difference Schemes For Wave Equation

2.1 Introduction

Propagation of waves at a high frequency or with large wave number is highly important as it finds applications in several walks of human life addressing their domestic, commercial, social and defence demands. Mathematically complex nature of these phenomenon poses a challenge to physicists, engineers, scientists and mathematicians to find explicit analytical solution, which are mostly tedious and in many situations even they are not realistically possible to calculate. From here a numerical analysts job starts, to make an impossible a *Possible* one. Consequently, numerical schemes are developed over the decades by many researchers for wave propagation problems, which fails to propagate waves at correct speed and results into errors namely, numerical dispersion also known as phase error and numerical dissipation also named as amplitude error. These errors arise because of the discrete nature of the numerical schemes, used to solve these problems. Researchers are interested in theoretically detailed understanding of the dispersive and dissipative properties of a numerical scheme because it serves as a priori error estimate for the practical problems. Several numerical schemes are reported by many $[13, 16, 17, 20, 22, 23, 25, 31, 32, 33, 34, 36, 37, 38]$, to reduce dispersion in one dimension as it is already proved that dispersion cannot be avoided for problems posed in higher dimensions.

Recently, Shu and Li [2] in 2010, presented an exact finite difference scheme for solving Helmholtz equation, with high wave number. They found a dispersion controlling parameter α, by redefining the standard second order central finite difference scheme, and made not only the C.F.D scheme exact but also made the non−reflecting boundary condition exact. They presented analysis of the novel scheme for a broad range of wave numbers. However, one can say that [2] is an extension of an idea of Nherbass and lee [1] introduced in 1998, but with a different approach. The value of α is same, but [1] does not work for high wave number, since here only the C.F.D scheme was made exact.

Sutmann [41] in 2007, derived a new compact finite difference scheme of sixth order for solving the Helmholtz equation, further discussing the convergence and accuracy for a large range of wave numbers. Yiping [10] in 2008, developed two fourth order accurate compact finite difference schemes for solving Helmholtz equation in two space dimensions for large wave number. In one of the schemes he succeeded to obtain an expression of truncation error independent of wave number, which made the scheme work well for large wave numbers. Whereas, Nabavi, Siddiqui and Dargahi [9] in 2007, proposed a new nine point sixth order accurate compact finite difference method for solving Helmholtz equation. Singer and Turkel [8] in 1998, constructed higher order method for Helmholtz equation in one and two dimensions with uniform grid.

Finkelstein [7] in 2009, derived explicit F.D.T.D dispersion reduction schemes for Maxwell's and wave equations in one and two dimensions. Other numerical techniques such as optimally blended scheme, spectral element scheme and finite element scheme $[13, 20, 22]$ are also developed to solve wave propagation problems.

2.2 Hyperbolic partial differential equations

In the first chapter, we introduced ourselves to different classes of second order partial differential equations, one of them is the hyperbolic partial differential equation. This usually arises when waves and vibrations occur in a physical system, and the mathematical modeling of such a system always involves the solution of a hyperbolic equation or a hyperbolic system. Here the equation of our interest is the transient wave equation defined in (1.6).

From the study of literature, we learned that different numerical schemes are extensively been used to simulate the wave propagation phenomena. But these numerical schemes suffer from numerical errors, dispersion and dissipation, because when we solve the problem numerically we have to shift it from a continuous level to a discrete level, by discretizing the domain. People have done a lot of work in time harmonic form of the wave equation, since it is an easier form to tackle with, whereas the time dependent wave equation is a bit difficult to handle, and not much work is done for this equation. There does not exist any optimal central finite difference scheme for the wave equation in literature, however there are other numerical schemes but usually these schemes suffer from a limitation to use a fine mesh in order to get an accurate solution, and some do not work for high wave number. Therefore, the objective of this thesis is to develop an accurate and at the same time an efficient numerical schemes, for transient wave equation, which are less dispersive and less dissipative.

In this research work we will optimize the transient wave equation, by developing the novel central finite difference schemes. Furthermore, we will implement the idea on a vibrating string problem and a wave propagation problem. We will discuss them one by one, and include the standard second order central finite difference schemes for comparison. We will also prove and show that the novel schemes give the exact values (meaning that very high accuracy) at the grid points and is almost an exact interpolant of the analytical solution. We will start the section by developing the optimal central finite difference schemes for one dimensional transient wave equation, that is

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \qquad x \in (a,b), t > 0. \tag{2.1}$$

2.2.1 Novel explicit scheme

We replace the partial derivatives, $\partial^2 u/\partial x^2$ and $\partial^2 u/\partial t^2$, present in (2.1), by the standard second order central finite difference approximation which involves α as a weight of the central node instead of 2, in order to form the novel explicit scheme. As follows,

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= \frac{1}{h^2}\left[u(x+h,t) - \alpha u(x,t) + u(x-h,t)\right], \\ \text{and} \quad \frac{\partial^2 u}{\partial t^2} &= \frac{1}{l^2}\left[u(x,t+l) - \alpha u(x,t) + u(x,t-l)\right]. \end{aligned}$$

Using these approximations in (2.1), we have

$$\frac{[u(x+h,t) - \alpha u(x,t) + u(x-h,t)]}{h^2} = \left(\frac{1}{c^2}\right)\frac{[u(x,t+l) - \alpha u(x,t) + u(x,t-l)]}{l^2}$$

further simplification gives,

$$(rc)^2[u(x+h,t) - \alpha u(x,t) + u(x-h,t)] = u(x,t+l) - \alpha u(x,t) + u(x,t-l) \tag{2.2}$$

where $r = (l/h)$. Here, in (2.2) α is unknown. In order to find the value α, we make use of the plane wave solution, that is $u(x,t) = e^{i(kx-\omega t)}$. From this we have the following definitions,

$$\begin{aligned} u(x+h,t) &= e^{i(k(x+h)-\omega t)} \\ u(x-h,t) &= e^{i(k(x-h)-\omega t)} \\ u(x,t+l) &= e^{i(kx-\omega(t+l))} \\ u(x,t-l) &= e^{i(kx-\omega(t-l))}. \end{aligned}$$

Using them in (2.2), we have

$$\begin{aligned}
(rc)^2[e^{i(k(x+h)-\omega t)} - \alpha e^{i(kx-\omega t)} + e^{i(k(x-h)-\omega t)}] &= [e^{i(kx-\omega(t+l))} - \alpha e^{i(kx-\omega t)} + e^{i(kx-\omega(t-l))}] \\
(rc)^2[e^{ikx}e^{ikh}e^{-i\omega t} - \alpha e^{ikx}e^{-i\omega t} + e^{ikx}e^{-ikh}e^{-i\omega t}] &= [e^{ikx}e^{-i\omega t}e^{-i\omega l} - \alpha e^{ikx}e^{-i\omega t} + e^{ikx}e^{-i\omega t}e^{i\omega l}] \\
(rc)^2(e^{ikh} + e^{-ikh} - \alpha)(e^{ikx}e^{-i\omega t}) &= (e^{i\omega l} + e^{-i\omega l} - \alpha)(e^{ikx}e^{-i\omega t}) \\
(rc)^2(2\cos(kh) - \alpha)e^{i(kx-\omega t)} &= (2\cos(\omega l) - \alpha)e^{i(kx-\omega t)} \\
(rc)^2(2\cos(kh) - \alpha)u(x,t) &= (2\cos(\omega l) - \alpha)u(x,t)
\end{aligned}$$

by just rearranging the above equation, we have

$$[2(rc)^2\cos(kh) - (rc)^2\alpha - 2\cos(\omega l) + \alpha]u(x,t) = 0.$$

As $u(x,t) \neq 0$, it implies that,

$$\begin{aligned}
2(rc)^2\cos(kh) - (rc)^2\alpha - 2\cos(\omega l) + \alpha &= 0 \\
2(rc)^2\cos(kh) - 2\cos(\omega l) - \alpha((rc)^2 - 1) &= 0 \\
\alpha((rc)^2 - 1) &= 2(rc)^2\cos(kh) - 2\cos(\omega l)
\end{aligned}$$

Finally, we have the value of α as

$$\alpha = \frac{2}{((rc)^2 - 1)}[(rc)^2\cos(kh) - \cos(\omega l)]. \tag{2.3}$$

Insert the value of α from (2.3) in (2.2), and after modification, we get the novel explicit C.F.D scheme as below.

$$\begin{aligned}
u(x,t+l) + u(x,t-l) &= r^2c^2[u(x+h,t) + u(x-h,t)] \\
&\quad +2[\cos(\omega l) - (rc)^2\cos(kh)]u(x,t)
\end{aligned} \tag{2.4}$$

or, we can write the required form of the novel explicit scheme, as follow

$$u_m^{n+1} = c^2r^2(u_{m+1}^n + u_{m-1}^n) + 2[\cos(\omega l) - (rc)^2\cos(kh)]u_m^n - u_m^{n-1}.$$

Interestingly, we can construct (2.4) by using a very powerful tool known as *bloch wave property.* Lets see how this works. By using Taylor's series expansion of $u(x+h,t)$ and $u(x-h,t)$, as

$$u(x+h,t) = u(x,t) + hu'(x,t) + \frac{h^2}{2!}u''(x,t) + \frac{h^3}{3!}u'''(x,t) + \frac{h^4}{4!}u^4(x,t) + \cdots$$

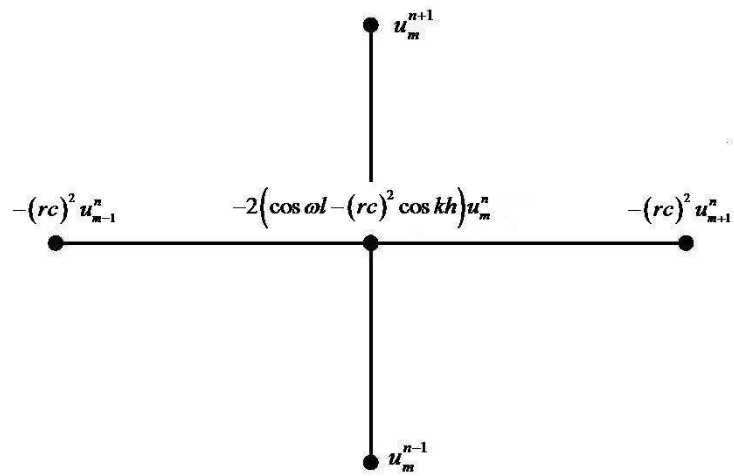

Figure 2.1: Stencil for novel explicit scheme.

and

$$u(x-h,t)=u(x,t)-hu'(x,t)+\frac{h^2}{2!}u''(x,t)-\frac{h^3}{3!}u'''(x,t)+\frac{h^4}{4!}u^4(x,t)-\cdots$$

adding the above two equations we have,

$$u(x+h,t)+u(x-h,t)=2\left[u(x,t)+\frac{h^2}{2!}u''(x,t)+\frac{h^4}{4!}u^4(x,t)+\cdots\right].$$

Use the plane wave solution $u(x,t)=e^{i(kx-\omega t)}$, to define $u''(x,t)$, $u^4(x,t)$, $\cdots$, and replace them in the above equation. We get the following form,

$$u(x+h,t)+u(x-h,t)=2\left[1-\frac{hk^2}{2!}+\frac{hk^4}{4!}+\cdots\right]u(x,t)$$

or, we can write it as

$$u(x+h,t)+u(x-h,t)=2\cos(hk)u(x,t) \tag{2.5}$$

using (2.5) in (2.2), and proceeding further in the same way as in the first method, we have the same value of α given in (2.3). Which finally gives the scheme (2.4). Next, to show that (2.4) is dispersion free, we insert a plane wave solution in it, of the form $u(x,t) = e^{i(\tilde{k}x-\omega t)}$, where $\tilde{k}$ is the numerical wave number, and have the following definitions.

$$\begin{aligned} u(x+h,t) &= e^{i(\tilde{k}(x+h)-\omega t)} \\ u(x-h,t) &= e^{i(\tilde{k}(x-h)-\omega t)} \\ u(x,t+l) &= e^{i(\tilde{k}x-\omega(t+l))} \\ u(x,t-l) &= e^{i(\tilde{k}x-\omega(t-l))} \end{aligned}$$

using them in (2.4), gives us

$$\begin{aligned} [e^{i(\tilde{k}x-\omega(t+l))} + e^{i(\tilde{k}x-\omega(t-l))}] &= (rc)^2[e^{i(\tilde{k}(x+h)-\omega t)} + e^{i(\tilde{k}(x-h)-\omega t)}] \\ &\quad -2[(rc)^2\cos(kh) - \cos(\omega l)]e^{i(\tilde{k}x-\omega t)} \\ (e^{i\omega l} + e^{-i\omega l})e^{i\tilde{k}x}e^{-i\omega t} &= (rc)^2[(e^{ikh} + e^{-ikh})e^{ikx}e^{-i\omega t}] \\ &\quad -2[(rc)^2\cos(kh) - \cos(\omega l)]e^{i(\tilde{k}x}e^{-i\omega t)} \\ 2\cos(\omega l)e^{i(\tilde{k}x-\omega t)} &= 2(rc)^2\cos(\tilde{k}h)e^{i(\tilde{k}x-\omega t)} - 2[(rc)^2\cos(kh) - \cos(\omega l)]e^{i(\tilde{k}x-\omega t)}. \end{aligned}$$

Rearranging further, we get

$$[\cos(\omega l) - (rc)^2\cos(\tilde{k}h) + (rc)^2\cos(kh) - \cos(\omega l)]e^{i(\tilde{k}x-\omega t)} = 0$$

$$[\cos(\omega l) - (rc)^2\cos(\tilde{k}h) + (rc)^2\cos(kh) - \cos(\omega l)]u(x,t) = 0.$$

As $u(x,t) \neq 0$, so it implies that,

$$\begin{aligned} \cos(\omega l) - (rc)^2\cos(\tilde{k}h) + (rc)^2\cos(kh) - \cos(\omega l) &= 0 \\ -(rc)^2\cos(\tilde{k}h) + (rc)^2\cos(kh) &= 0 \\ \cos(\tilde{k}h) &= \cos(kh) \\ \tilde{k}h &= kh \\ \text{or} \quad \tilde{k} - k &= 0. \end{aligned}$$

This is the desired situation, indicating that the novel explicit scheme (2.4), does not suffer from numerical dispersion.

2.2.2 Novel implicit scheme

Similarly, we have developed the implicit scheme for (2.1). This time we substitute $\partial^2 u/\partial t^2$, by its standard second order central finite difference approximation, involving 2 as the weight of the central node. Whereas, we substitute $\partial^2 u/\partial x^2$ by its weighted average, involving α as a weight of the central node instead of 2, they are defined as follows

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

and

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} = \frac{1}{4h^2}\Bigg\{ & u(x+h,t+l) - \alpha u(x,t+l) + u(x-h,t+l) + 2u(x+h,t) \\ & - 2\alpha u(x,t) + 2u(x-h,t) + u(x+h,t-l) - \alpha u(x,t-l) + u(x-h,t-l)\Bigg\}.\end{aligned}$$

Using these approximations in (2.1), we have

$$\begin{aligned}\frac{1}{4h^2}\Bigg\{ & u(x+h,t+l) - \alpha u(x,t+l) + u(x-h,t+l) + 2u(x+h,t) \\ & - 2\alpha u(x,t) + 2u(x-h,t) + u(x+h,t-l) - \alpha u(x,t-l) + u(x-h,t-l)\Bigg\} \\ & = \left(\frac{1}{c^2}\right)\frac{[u(x,t+l) - 2u(x,t) + u(x,t-l)]}{l^2}\end{aligned}$$

further simplifying the above equation, we obtain

$$\begin{aligned}\frac{(rc)^2}{4}\Bigg\{ & u(x+h,t+l) - \alpha u(x,t+l) + u(x-h,t+l) + 2u(x+h,t) \\ & - 2\alpha u(x,t) + 2u(x-h,t) + u(x+h,t-l) - \alpha u(x,t-l) + u(x-h,t-l)\Bigg\} \\ & = u(x,t+l) - 2u(x,t) + u(x,t-l) \quad (2.6)\end{aligned}$$

where $r = (l/h)$. Here α is unknown, in order to find the value α we make use of plane wave solution, that is $u(x,t) = e^{i(kx-\omega t)}$. From this we define $u(x+h,t+l)$,

$u(x-h,t+l)$, $u(x+h,t-l)$, $u(x-h,t-l)$, $u(x+h,t)$, $u(x-h,t)$, $u(x,t+l)$, and $u(x,t-l)$, in the similar manner as defined in the case of explicit scheme. Ultimately using them in (2.2), we have the following form.

$$\frac{(rc)^2}{4}\Big\{e^{i(k(x+h)-\omega(t+l))} - \alpha e^{i(kx-\omega(t+l))} + e^{i(k(x-h)-\omega(t+l))} + 2e^{i(k(x+h)-\omega t)}$$
$$- 2\alpha e^{i(kx-\omega t)} + 2e^{i(k(x-h)-\omega t)} + e^{i(k(x+h)-\omega(t-l))} - \alpha e^{i(kx-\omega(t-l))} + e^{i(k(x-h)-\omega(t-l))}\Big\}$$
$$= e^{i(kx-\omega(t+l))} - 2e^{i(kx-\omega t)} + e^{i(kx-\omega(t-l))}$$

simplifying it further

$$\frac{(rc)^2}{4}e^{i(kx-\omega t)}\Big\{e^{-ikh}e^{-i\omega l} - \alpha e^{-i\omega l} + e^{ikh}e^{-i\omega l} + 2e^{-ikh} - 2\alpha + 2e^{ikh}$$
$$+ e^{-ikh}e^{i\omega l} - \alpha e^{i\omega l} + e^{ikh}e^{i\omega l}\Big\} = e^{i(kx-\omega t)}[e^{i\omega l} - 2 + e^{-i\omega l}].$$

Rearranging the above equation, we have

$$\frac{(rc)^2}{4}\Big\{[e^{ikh} + e^{-ikh}][e^{i\omega l} + e^{-i\omega l}] - \alpha[e^{i\omega l} + e^{-i\omega l} + 2]$$
$$+ 2[e^{ikh} + e^{-ikh}]\Big\}e^{i(kx-\omega t)} - [e^{i\omega l} + e^{-i\omega l} - 2]e^{i(kx-\omega t)} = 0$$

or, we can write it as follows

$$\Big\{\frac{(rc)^2}{4}[4\cos(kh)\cos(\omega l) - 2\alpha(\cos(\omega l)+1) + 4\cos(kh)]$$
$$- 2(\cos(\omega l) - 1)\Big\}u(x,t) = 0.$$

As $u(x,t) \neq 0$, it implies that,

$$\frac{(rc)^2}{4}[4\cos(kh)\cos(\omega l) - 2\alpha(\cos(\omega l)+1) + 4\cos(kh)] - 2(\cos(\omega l) - 1) = 0$$

$$\frac{(rc)^2}{2}\alpha(\cos(\omega l)+1) = (rc)^2\cos(kh)\cos(\omega l) + (rc)^2\cos(kh) - 2(\cos(\omega l) - 1)$$

consequently, we have

$$\begin{aligned}\alpha &= \frac{2}{(rc)^2(\cos(\omega l)+1)}\left[(rc)^2\cos(kh)(\cos(\omega l)+1)-2(\cos(\omega l)-1)\right]\\ \text{or}\quad \alpha &= 2\left[\cos(kh)-\frac{2(\cos(\omega l)-1)}{(rc)^2(\cos(\omega l)+1)}\right],\ \text{ and }\ (rc)^2(\cos(\omega l)+1)\neq 0.\end{aligned}$$

Therefore the value of α is,

$$\alpha = 2\cos(kh)-\frac{4(\cos(\omega l)-1)}{(rc)^2(\cos(\omega l)+1)}. \tag{2.7}$$

Now, insert the value of α from (2.7), in (2.6), after simplification, we get the novel implicit C.F.D scheme as;

$$\begin{aligned}-\frac{(rc)^2}{4}\left[u(x-h,t+l)+u(x+h,t+l)\right]+\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]u(x,t+l)\\ =\frac{(rc)^2}{2}\left[u(x+h,t)+u(x-h,t)\right]+\frac{(rc)^2}{4}\left[u(x+h,t-l)+u(x-h,t-l)\right]\\ +\left[2-(rc)^2\cos(kh)-2\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]u(x,t)\\ -\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]u(x,t-l). \tag{2.8}\end{aligned}$$

We can write the required form of the implicit scheme, as follows

$$\begin{aligned}-\frac{(rc)^2}{4}\left[u_{m-1}^{n+1}+u_{m+1}^{n+1}\right]+\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]u_m^{n+1}\\ =\frac{(rc)^2}{2}\left[u_{m+1}^{n}+u_{m-1}^{n}\right]+\frac{(rc)^2}{4}\left[u_{m+1}^{n-1}+u_{m-1}^{n-1}\right]\\ +\left[2-(rc)^2\cos(kh)-2\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]u_m^{n}\\ -\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]u_m^{n-1}.\end{aligned}$$

Similarly, we can construct (2.8) by using the *bloch wave property*. Again by using Taylor's series expansion, we can define the following

$$u(x+h,t+l)+u(x-h,t+l)=2\cos(hk)u(x,t+l) \tag{2.9}$$

$$u(x+h,t-l)+u(x-h,t-l)=2\cos(hk)u(x,t-l) \tag{2.10}$$

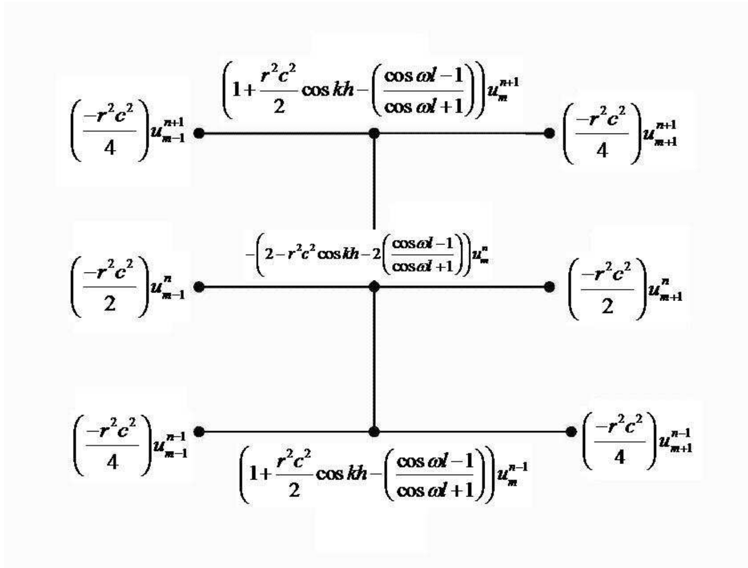

Figure 2.2: Stencil for novel implicit scheme.

using (2.9), (2.5) and (2.10) in (2.6), and proceeding further in the same way, we have the same value of α given in (2.7). Which finally gives the scheme (2.8).
In order to show that (2.8) is dispersion free, we define the dispersion relation for the implicit scheme. Since, the plane wave solution is of the form $u(x,t) = e^{i(\tilde{k}x-\omega t)}$, where $\tilde{k}$ is the numerical wave number. From this we have the definitions of $u(x-h,t+l)$, $u(x-h,t-l)$, $u(x+h,t-l)$, $u(x+h,t+l)$, $u(x,t+l)$, $u(x+h,t)$, $u(x-h,t)$ and $u(x,t-l)$, in the same manner we had in the case of explicit scheme. So, using them in (2.8), gives us

$$\begin{aligned}
&-\frac{(rc)^2}{4}\left[e^{i(\tilde{k}(x-h)-\omega(t+l))}+e^{i(\tilde{k}(x+h)-\omega(t+l))}\right]\\
&+\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{i(\tilde{k}x-\omega(t+l))}\\
&=\frac{(rc)^2}{2}\left[e^{i(\tilde{k}(x-h)-\omega t)}+e^{i(\tilde{k}(x+h)-\omega t)}\right]\\
&+\frac{(rc)^2}{4}\left[e^{i(\tilde{k}(x-h)-\omega(t-l))}+e^{i(\tilde{k}(x+h)-\omega(t-l))}\right]\\
&+\left[2-(rc)^2\cos(kh)+2\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{i(\tilde{k}x-\omega t)}\\
&-\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{i(\tilde{k}x-\omega(t-l))}
\end{aligned}$$

keep modifying it,

$$\left\{-\frac{(rc)^2}{4}\left[e^{-i\tilde{k}h}e^{-i\omega l}+e^{i\tilde{k}h}e^{-i\omega l}\right]+\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{-i\omega l}\right\}e^{i(\tilde{k}x-\omega t)}$$
$$=\left\{\frac{(rc)^2}{2}\left[e^{-i\tilde{k}h}+e^{i\tilde{k}x}\right]+\frac{(rc)^2}{4}\left[e^{-i\tilde{k}h}e^{i\omega l}+e^{i\tilde{k}h}e^{i\omega l}\right]\right.$$
$$\left.+2\left[1-\frac{(rc)^2}{2}\cos(kh)+\frac{(\cos(\omega l)-1)}{(\cos(\omega l)+1)}\right]-\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{i\omega l}\right\}e^{i(\tilde{k}x-\omega t)}$$

as $e^{i(\tilde{k}x-\omega t)}=u(x,t)\neq 0$, it implies that

$$-\frac{(rc)^2}{4}\left[e^{-i\tilde{k}h}e^{-i\omega l}+e^{i\tilde{k}h}e^{-i\omega l}\right]+\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{-i\omega l}$$
$$-\frac{(rc)^2}{2}\left[e^{-i\tilde{k}h}+e^{i\tilde{k}x}\right]-\frac{(rc)^2}{4}\left[e^{-i\tilde{k}h}e^{i\omega l}+e^{i\tilde{k}h}e^{i\omega l}\right]$$
$$-2\left[1-\frac{(rc)^2}{2}\cos(kh)+\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]+\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]e^{i\omega l}=0$$

further simplifying and rearranging the above equation, we get

$$-(rc)^2\cos(\tilde{k}h)\cos(\omega l)+2\left[1+\frac{(rc)^2}{2}\cos(kh)-\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]\cos(\omega l)$$
$$-(rc)^2\cos(\tilde{k}h)-2\left[1-\frac{(rc)^2}{2}\cos(kh)+\frac{\cos(\omega l)-1}{\cos(\omega l)+1}\right]=0$$

$$(rc)^2(\cos(\omega l)+1)(-\cos(\tilde{k}h)+\cos(kh))=0$$

since $(rc)^2(\cos(\omega l)+1)\neq 0$, it means that

$$\begin{aligned}-\cos(\tilde{k}h)+\cos(kh) &= 0\\ \cos(\tilde{k}h) &= \cos(kh)\\ \tilde{k}h &= kh\\ \text{or}\quad \tilde{k}-k &= 0.\end{aligned}$$

This is the desired situation, indicating that the novel implicit scheme (2.8), do not suffer from numerical dispersion.

2.2.3 Combined representation of novel explicit and implicit schemes

We can write both the novel explicit and implicit schemes in a compact form, by introducing parameter a. The benefit of this form is that, by just giving the value to a, we will get the desired scheme. Thus, the general representation for internal nodes, that is for $m = 1, 2, 3, ..., N-1.$ and $n = 1, 2, 3, ...,$ is as follows,

$$
\begin{aligned}
&-(rc)^2 a u_{m-1}^{n+1} + \left\{ 1 + a \left(2(rc)^2 \cos(kh) - 4 \left[\frac{\cos(\omega l) - 1}{\cos(\omega l) - 1} \right] \right) \right\} u_m^{n+1} \\
&\quad - (rc)^2 a u_{m+1}^{n+1} = -(rc)^2(-1 + 2a) u_{m-1}^{n} + \Bigg\{ 8a + 2(-1 + 3a)(rc)^2 \cos(kh) + \\
&\qquad 2(1 - 4a)\cos(\omega l) + 8a \left[\frac{\cos(\omega l) - 1}{\cos(\omega l) + 1} \right] \Bigg\} u_m^{n} - (rc)^2(-1 + 2a) u_{m+1}^{n} \\
&\qquad\qquad + (rc)^2 a (u_{m-1}^{n-1} + u_{m+1}^{n-1}) \\
&\qquad\qquad - \left\{ 1 + a \left(2(rc)^2 \cos(kh) - 4 \left[\frac{\cos(\omega l) - 1}{\cos(\omega l) + 1} \right] \right) \right\} u_m^{n-1}.
\end{aligned}
$$

If we substitute $a = 0$, in this form, we will get the explicit scheme (2.4). On the other hand if we substitute $a = (1/4)$, in this, we will get the implicit scheme (2.8).

The following are few very important traits of the novel schemes.

1. they are based upon a simple idea;

2. they are in more general form, and we can go back to standard ones by expanding $\cos(kh)$ and $\cos(\omega l)$ to a single term;

3. they are dispersion free and give optimal results;

4. there is no need to write new codes altogether, just correct the middle node of the standard codes, meaning that the implementation of novel schemes require no additional cost;

5. they work for any wave number k, small as well as large, but specifically they are designed for large wave numbers;

6. they do not require to use fine mesh size and;

7. one need to know the exact solution before hand.

In order to give the practical proof of our work, we have implemented the idea on two model problems. The first one is the vibrating string problem, having Dirichlet boundary conditions at both ends, we will attempt it with explicit scheme as well as with implicit scheme to show that both schemes work for real problems. The second one is wave propagation problem, having Dirichlet at first end and Robin boundary condition at the other end, we will just solve it with explicit scheme. We will study them one by one, further making their analysis and comparison with the standard schemes, accompanied by graphs and tables.

2.2.4 First model problem: vibrating string

Consider the initial boundary value problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \tag{2.11}$$

defined in the (x, t) plane and region $R = [0 < x < 1] * [t > 0]$, with boundary ∂R together with the boundary conditions,

$$u(0, t) = u(1, t) = 0 \qquad t > 0 \tag{2.12}$$

and initial conditions

$$u(x, 0) = \sin(\pi x) \ \textit{and} \ \frac{\partial u(x, 0)}{\partial t} = 0 \qquad 0 \leq x \leq 1. \tag{2.13}$$

The exact solution of this problem is,

$$u(x, t) = \sin(\pi x)\cos(\pi t). \tag{2.14}$$

This describes an example of vibrating string, having both ends tied, with initial displacement defined by, $\sin(\pi x)$ and initial velocity given as zero. Here in this problem the propagation speed is taken as, $c^2 = 1$. The boundary conditions at $x = 0$ (origin) and at $x = 1$ holds for arbitrary t and similarly the initial conditions at $t = 0$ holds for $0 \leq x \leq 1$. We can observe clearly the continuity between the initial and the boundary condition at origin, since $u(0, 0) = 0$. We have discretized our domain, the interval $[0, 1]$ is divided into N subintervals each having the constant width h, given by $h = 1/(N)$ and similarly the time, $t \geq 0$ is divided into equal time steps of length l. Hence, we can write $x_m = mh$, and $t_n = nl$. Therefore, each node has coordinates of the following form.
$(x_m, t_n) = (mh, nl)$
with $m = 0, 1, 2, \cdots, N$ and $n = 0, 1, 2, \cdots$.
The region R, is an open rectangle bounded by $x = 0$, $x = 1$ and $t = 0$, further it is covered by a grid consisting of lines parallel to the time axis (t$-$axis) and the lines parallel to the space axis (x$-$axis).

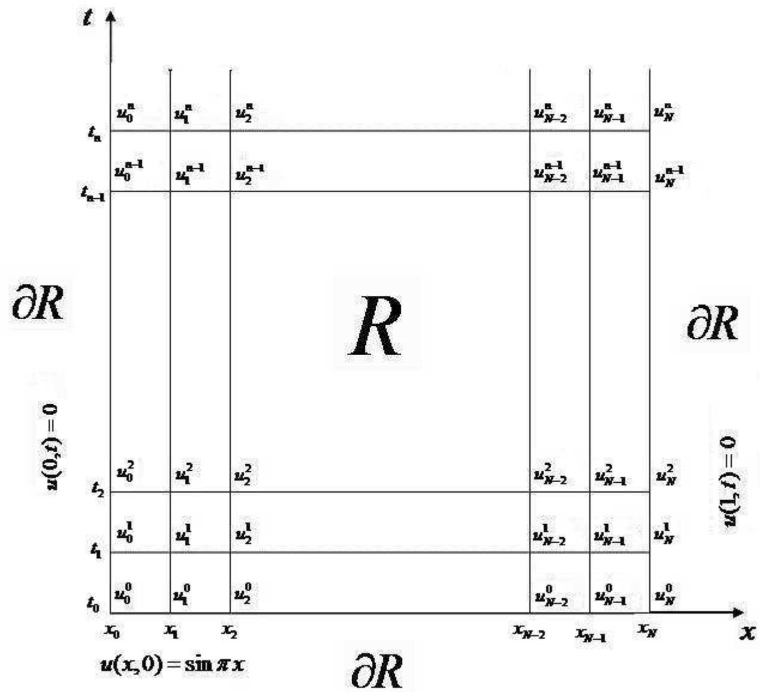

Figure 2.3: Domain of the first problem.

2.2.4.1 Model problem one: standard second order explicit C.F.D scheme

First of all, we will construct the standard second order central finite difference explicit scheme for the vibrating string problem. Therefore, replace the spatial derivative, $\partial^2 u/\partial x^2$ and the temporal derivative, $\partial^2 u/\partial t^2$ in (2.11) by their second order central finite difference approximations, they are defined as,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{h^2}\left[u(x+h,t) - 2u(x,t) + u(x-h,t)\right] + O(h^2), \tag{2.15}$$

and

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{l^2}\left[u(x,t+l) - 2u(x,t) + u(x,t-l)\right] + O(l^2). \tag{2.16}$$

Using (2.15) and (2.16) in (2.11), we get

$$\begin{aligned} \frac{1}{l^2}\left[u(x,t+l) - 2u(x,t) + u(x,t-l)\right] &= \frac{1}{h^2}\left[u(x+h,t) - 2u(x,t) + u(x-h,t)\right] \\ u(x,t+l) - 2u(x,t) + u(x,t-l) &= r^2[u(x+h,t) - 2u(x,t) + u(x-h,t)] \end{aligned}$$

with, $r^2 = (l/h)^2$.

Rewriting above equation, gives us

$$u(x,t+l) = 2(1-r^2)u(x,t) + r^2[u(x+h,t) + u(x-h,t)] - u(x,t-l)$$

or, we can write it as follows

$$u_m^{n+1} = 2(1-r^2)u_m^n + r^2(u_{m+1}^n + u_{m-1}^n) - u_m^{n-1}. \tag{2.17}$$

This is the standard second order explicit central finite difference, five point, three time level scheme for the defined first problem [4].

2.2.4.2 Standard second order implicit C.F.D scheme

In order to make the implicit scheme we have to use the weighted average approximation for $\partial^2 u/\partial x^2$, that is

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{4h^2}\Big\{u(x+h,t+l) - 2u(x,t+l) + u(x-h,t+l) + 2u(x+h,t)$$
$$-4u(x,t) + 2u(x-h,t) + u(x+h,t-l) - 2u(x,t-l) + u(x-h,t-l)\Big\} + O(h^2) \tag{2.18}$$

and standard approximation for $\partial^2 u/\partial t^2$, using (2.18) and (2.16) in (2.11), we get

$$\frac{1}{l^2}\Big\{u(x,t+l) - 2u(x,t) + u(x,t-l)\Big\} = \frac{1}{h^2}\Big\{u(x+h,t+l) - 2u(x,t+l)$$
$$+ u(x-h,t+l) + u(x+h,t) - 2u(x,t) + u(x-h,t)$$
$$+ u(x+h,t-l) - 2u(x,t-l) + u(x-h,t-l)\Big\}$$

simplifying further,

$$u(x,t+l) - 2u(x,t) + u(x,t-l) = \frac{r^2}{4}\Big\{u(x+h,t+l) - 2u(x,t+l)$$
$$+u(x-h,t+l)+2u(x+h,t)-4u(x,t)+2u(x-h,t)+u(x+h,t-l)-2u(x,t-l)+u(x-h,t-l)\Big\}$$

with $r^2 = (l/h)^2$. Gathering same terms, gives us

$$\begin{aligned} -\frac{r^2}{4}\left[u(x+h,t+l) + u(x-h,t+l)\right] \\ +\left(1+\frac{r^2}{2}\right)u(x,t+l) = (2-r^2)u(x,t) - \left(1+\frac{r^2}{2}\right)u(x,t-l) \\ +\frac{r^2}{2}\left(u(x+h,t) + u(x-h,t)\right) \\ +\frac{r^2}{4}\left(u(x+h,t-l) + u(x-h,t-l)\right) \end{aligned}$$

or, we can write it as follows

$$-\frac{r^2}{4}\left(u_{m+1}^{n+1} + u_{m-1}^{n+1}\right) + \left(1+\frac{r^2}{2}\right)u_m^{n+1} = (2-r^2)u_m^n - (1+\frac{r^2}{2})u_m^{n-1}$$

$$+\frac{r^2}{2}\left(u_{m-1}^{n}+u_{m+1}^{n}\right)+\frac{r^2}{4}\left(u_{m+1}^{n-1}+u_{m-1}^{n-1}\right). \tag{2.19}$$

This is the standard second order implicit central finite difference, nine point, three time level scheme for the first problem [4].

2.2.4.3 Solution at first time step

This subsection has the purpose to calculate the value of $u(x,t)$, at first time step. Since, it is not explicitly contained in the initial conditions. So, we need a sufficiently accurate approximation to the dependent variable at the first time step, to be used in (2.17) and (2.19). Here, we make use of initial velocity given in (2.13), that is

$$\frac{\partial u}{\partial t}=0.$$

Now, replace the partial derivative with its second order finite difference approximation, we get

$$\frac{u(x,t+l)-u(x,t-l)}{2l}=0$$

$$u(x,t-l)=u(x,t+l). \tag{2.20}$$

Using (2.20) in (2.17), we have the following scheme

$$u_m^{n+1}=(1-r^2)u_m^n+\frac{r^2}{2}(u_{m-1}^{n}+u_{m+1}^{n})$$

to calculate the solution at first time step for explicit system. Similarly, using (2.20) in (2.19), will give us the following scheme to compute the solution at first time step of implicit system.

$$-\frac{r^2}{4}\left(u_{m+1}^{n+1}+u_{m-1}^{n+1}\right)+2\left(1+\frac{r^2}{2}\right)u_m^{n+1}=(2-r^2)u_m^n$$
$$+\frac{r^2}{2}\left(u_{m-1}^{n}+u_{m+1}^{n}\right)+\frac{r^2}{4}\left(u_{m+1}^{n-1}+u_{m-1}^{n-1}\right).$$

2.2.4.4 Full system for second order standard explicit C.F.D scheme

The full system for the first problem is given below

$$\text{at } \ m = 0, n = 0, 1, 2, \cdots$$

$$u_m^n = 0,$$

$$\text{at } \ m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^n = \sin(mh\pi),$$

$$\text{at } \ m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^{n+1} = (1-r^2)u_m^n + \frac{r^2}{2}(u_{m-1}^n + u_{m+1}^n)$$

$$\text{at } \ m = 1, 2, \cdots, N-1, n = 1, 2, \cdots$$

$$u_m^{n+1} = 2(1-r^2)u_m^n + r^2(u_{m-1}^n + u_{m+1}^n) - u_m^{n-1}$$

$$\text{at } \ m = N, n = 0, 1, 2 \cdots$$

$$u_m^n = 0.$$

2.2.4.5 Full system for second order standard implicit C.F.D scheme

The full system for the first problem is given below

$$
\begin{aligned}
&\text{at } m=0, n=0,1,2,\cdots\\
&u_m^n=0,\\
&\text{at } m=1,2,\cdots,N-1, n=0\\
&u_m^n=\sin(mh\pi),\\
&\text{at } m=1,2,\cdots,N-1, n=0\\
-\frac{r^2}{4}\left(u_{m+1}^{n+1}+u_{m-1}^{n+1}\right)+2\left(1+\frac{r^2}{2}\right)u_m^{n+1}&=(2-r^2)u_m^n\\
&+\frac{r^2}{2}\left(u_{m-1}^n+u_{m+1}^n\right)+\frac{r^2}{4}\left(u_{m+1}^{n-1}+u_{m-1}^{n-1}\right)\\
&\text{at } m=1,2,\ldots,N-1, n=1,2,\cdots\\
-\frac{r^2}{4}\left(u_{m+1}^{n+1}+u_{m-1}^{n+1}\right)+\left(1+\frac{r^2}{2}\right)u_m^{n+1}&=(2-r^2)u_m^n-(1+\frac{r^2}{2})u_m^{n-1}\\
&+\frac{r^2}{2}\left(u_{m-1}^n+u_{m+1}^n\right)+\frac{r^2}{4}\left(u_{m+1}^{n-1}+u_{m-1}^{n-1}\right)\\
&\text{at } m=N, n=0,1,2,\cdots\\
&u_m^n=0.
\end{aligned}
$$

2.2.4.6 Combined representation of standard second order explicit and implicit C.F.D schemes for first problem

We can write both the schemes in a combined form, with the help of parameter a, [4]. So that by just giving specific value to a, result into the desired scheme either explicit or implicit. So, the general representation for the first time step is,

$$\begin{aligned} -r^2a(u^{n+1}_{m+1}+u^{n+1}_{m-1})+2(1+2r^2a)u^{n+1}_m \\ = 2(1+2r^2a-r^2)u^n_m+r^2(1-2a)[u^n_{m-1}+u^n_{m+1}] \\ +r^2a[u^{n-1}_{m+1}+u^{n-1}_{m-1}] \end{aligned}$$

insert $a=0$ and $a=1/4$, it will yield the explicit and implicit, first time step schemes respectively. Similarly, for internal nodes we have,

$$\begin{aligned} -r^2a(u^{n+1}_{m+1}+u^{n+1}_{m-1})+(1+2r^2a)u^{n+1}_m \\ = 2(1+2r^2a-r^2)u^n_m+r^2(1-2a)[u^n_{m-1}+u^n_{m+1}] \\ +r^2a[u^{n-1}_{m+1}+u^{n-1}_{m-1}]-(1+2r^2a)u^{n-1}_m \end{aligned}$$

where $a>0$. Note that, to obtain the explicit scheme (2.17), we insert $a=0$ and to have the implicit scheme (2.19), we insert $a=1/4$ in the above equation.

2.2.4.7 Construction of novel explicit C.F.D scheme for model problem one

In this section, we will construct the novel explicit scheme for the vibrating string problem, rewritten below

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \qquad 0 < x < 1, t > 0$$

$$u(0,t) = u(1,t) = 0 \qquad t > 0$$

$$u(x,0) = \sin(\pi x), \quad \frac{\partial u(x,0)}{\partial t} = 0 \qquad 0 \le x \le 1.$$

To achieve our target, this time we will replace the partial derivatives $\partial^2 u/\partial x^2$ and $\partial^2 u/\partial t^2$, in the governing differential equation, by the following.

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

and

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{l^2}\left[u(x,t+l) - \alpha u(x,t) + u(x,t-l)\right] + O(l^2).$$

Here, the standard C.F.D approximations for spatial as well as the temporal part are modified by assigning α as a weight of the central node, instead of 2. After using these substitutions in the equation (2.11), we have the form.

$$u(x,t+l) - \alpha u(x,t) + u(x,t-l) = r^2[u(x+h,t) - \alpha u(x,t) + u(x-h,t)] \quad (2.21)$$

where $r = l/h$. As α is unknown above, so the second step is to find the value of this α. Therefore, consider the exact solution, u(x,t)=$\sin(\pi x)\cos(\pi t)$, and define the following.

$$\begin{aligned} u(x+h,t) &= \sin(\pi(x+h))\cos(\pi t) \\ u(x-h,t) &= \sin(\pi(x-h))\cos(\pi t) \\ u(x,t+l) &= \sin(\pi x)\cos(\pi(t+l)) \\ \text{and} \quad u(x,t-l) &= \sin(\pi x)\cos(\pi(t-l)). \end{aligned}$$

Using these substitutions in (2.21), we have

$$\sin(\pi x)\cos(\pi(t-l)) - \alpha\sin(\pi x)\cos(\pi t) + \sin(\pi x)\cos(\pi(t+l))$$
$$= r^2[\sin(\pi(x-h))\cos(\pi t) - \alpha\sin(\pi x)\cos(\pi t) + \sin(\pi(x+h))\cos(\pi t)]$$

after simplification we are left with,

$$\begin{aligned} [2\cos(\pi l) - \alpha - 2r^2\cos(\pi h) + \alpha r^2]\sin(\pi x)\cos(\pi t) &= 0 \\ \text{or} \quad [2\cos(\pi l) - \alpha - 2r^2\cos(\pi h) + \alpha r^2]u(x,t) &= 0. \end{aligned}$$

Since, we know that $u(x,t) \neq 0$. It means that

$$2\cos(\pi l) - \alpha - 2r^2\cos(\pi h) + \alpha r^2 = 0$$
$$\text{or} \quad \alpha(r^2-1) + 2\cos(\pi l) - 2r^2\cos(\pi h) = 0.$$

Rearranging the above expression to get the value of α

$$\alpha = \frac{2}{1-r^2}\left(\cos(\pi l) - r^2\cos(\pi h)\right). \tag{2.22}$$

Substituting the value of α from (2.22), in (2.21) and performing ordinary simplifications result into the following five point, two time level novel explicit scheme

$$u(x,t+l) = 2[\cos(\pi l) - r^2\cos(\pi h)]u(x,t) + r^2[u(x-h,t) + u(x+h,t)] - u(x,t-l) \tag{2.23}$$

or in another form, we can write it as

$$u_m^{n+1} = 2[\cos(\pi l) - r^2\cos(\pi h)]u_m^n + r^2(u_{m-1}^n + u_{m+1}^n) - u_m^{n-1}.$$

In the next step, we are going to check the exactness of novel scheme (2.23). To do so, we apply the scheme, (2.23) on (mh, nl) nodes. Now, since we know that $u(x,t) = \sin(\pi x)\cos(\pi t)$, it gives $u(mh, nl) = \sin(mh\pi)\cos(nl\pi)$. Similarly, we can define it for $u((m+1)h, nl)$, $u((m-1)h, nl)$, $u(mh, (n+1)l)$ and $u(mh, (n-1)l)$. The scheme (2.23), when applied at (mh, nl), gives after rearranging

$$\begin{aligned} \sin(mh\pi)\cos((n+1)l\pi) - 2[\cos(l\pi) - r^2\cos(h\pi)]\sin(mh\pi)\cos(nl\pi) \\ -r^2[\sin((m+1)h\pi)\cos(nl\pi) + \sin((m-1)h\pi)\cos(nl\pi)] \\ +\sin(mh\pi)\cos((n-1)l\pi) = 0 \end{aligned}$$

further we have,

$$\begin{aligned}
&\sin(mh\pi)\cos(nl\pi)\cos(l\pi)-\sin(mh\pi)\sin(nl\pi)\sin(l\pi)\\
&-2\cos(l\pi)\sin(mh\pi)\cos(nl\pi)+2r^2\cos(h\pi)\sin(mh\pi)\cos(nl\pi)\\
&-r^2\sin(mh\pi)\cos(h\pi)\cos(nl\pi)-r^2\sin(h\pi)\cos(mh\pi)\cos(nl\pi)\\
&-r^2\sin(mh\pi)\cos(h\pi)\cos(nl\pi)+r^2\sin(h\pi)\cos(mh\pi)\cos(nl\pi)\\
&+\sin(mh\pi)\cos(nl\pi)\cos(l\pi)+\sin(mh\pi)\sin(nl\pi)\sin(l\pi)=0.
\end{aligned}$$

All the terms will be canceled making $L.H.S = R.H.S = 0$, which proves the exactness of (2.23). Therefore, novel explicit scheme (2.23) is dispersion free.

2.2.4.8 Construction of novel implicit C.F.D scheme for model problem one

Reconsider the vibrating string problem, defined in (2.11) along with the initial conditions given in (2.13) and boundary conditions (2.12), whereas the exact solution is presented in (2.14). We are going to construct the implicit scheme for this problem.

Replace the spatial partial derivative, $\partial^2u/\partial x^2$ by its weighted average with central node weight α instead of 2 and the temporal partial derivative, $\partial^2u/\partial t^2$ with its standard second order approximation which do not involve α with its central node. That is

$$\frac{\partial^2u}{\partial x^2}=\frac{1}{4h^2}\Big\{u(x+h,t+l)-\alpha u(x,t+l)+u(x-h,t+l)+2u(x+h,t)$$
$$-2\alpha u(x,t)+2u(x-h,t)+u(x+h,t-l)-\alpha u(x,t-l)+u(x-h,t-l)\Big\}$$

$$\text{and}\quad \frac{\partial^2u}{\partial t^2}=\frac{1}{l^2}\left[u(x,t+l)-2u(x,t)+u(x,t-l)\right]$$

replacing them in (2.11), this gives us after rearranging

$$\begin{aligned}
-\frac{r^2}{4}\left[u(x+h,t+l)+u(x-h,t+l)\right]+\left(1+\alpha\frac{r^2}{4}\right)u(x,t+l)\\
=\frac{r^2}{2}\left[u(x+h,t)+u(x-h,t)\right]+\left(2-\alpha\frac{r^2}{2}\right)u(x,t)
\end{aligned}$$

$$+\frac{r^2}{4}\left[u(x+h,t-l)+u(x-h,t-l)\right]-\left(1+\alpha\frac{r^2}{4}\right)u(x,t-l) \tag{2.24}$$

where $r = l/h$. It remains to find the value of α, in the novel scheme. For this we need the aid of an exact solution defined in (2.14). Consider now the exact solution

$$u(x,t) = \sin(\pi x)\cos(\pi t)$$

along with the following

$$\begin{aligned}
u(mh,nl) &= \sin(mh\pi)\cos(nl\pi)\\
u((m+1)h,nl) &= \sin((m+1)h\pi)\cos(nl\pi)\\
u((m-1)h,nl) &= \sin((m-1)h\pi)\cos(nl\pi)\\
u(mh,(n+1)l) &= \sin(mh\pi)\cos((n+1)l\pi)\\
u(mh,(n-1)l) &= \sin(mh\pi)\cos((n-1)l\pi)\\
u((m+1)h,(n+1)l) &= \sin((m+1)h\pi)\cos((n+1)l\pi)\\
u((m-1)h,(n+1)l) &= \sin((m-1)h\pi)\cos((n+1)l\pi)\\
u((m+1)h,(n-1)l) &= \sin((m+1)h\pi)\cos((n-1)l\pi)\\
u((m-1)h,(n-1)l) &= \sin((m-1)h\pi)\cos((n-1)l\pi).
\end{aligned}$$

Making use of the above nine equations, in (2.24), we have the next equation

$$\begin{aligned}
-\frac{r^2}{4}\sin((m+1)h\pi)\cos((n+1)l\pi)-\frac{r^2}{4}\sin((m-1)h\pi)\cos((n+1)l\pi)\\
+\sin(mh\pi)\cos((n+1)l\pi)+\alpha\frac{r^2}{4}\sin(mh\pi)\cos((n+1)l\pi)=2\sin(mh\pi)\cos(nl\pi)\\
+\frac{r^2}{2}\sin((m-1)h\pi)\cos(nl\pi)+\frac{r^2}{2}\sin((m+1)h\pi)\cos(nl\pi)\\
-\alpha\frac{r^2}{2}\sin(mh\pi)\cos(nl\pi)-\sin(mh\pi)\cos((n-1)l\pi)\\
+\frac{r^2}{4}\sin((m+1)h\pi)\cos((n-1)l\pi)+\frac{r^2}{4}\sin((m-1)h\pi)\cos((n-1)l\pi)\\
-\alpha\frac{r^2}{4}\sin(mh\pi)\cos((n-1)l\pi)
\end{aligned}$$

after simplifying we are left with,

$$-2\cos(l\pi)+2+r^2\cos(h\pi)\cos(l\pi)+r^2\cos(h\pi)=\alpha\frac{r^2}{2}(\cos(l\pi)+1)$$

$$\text{or} \quad \alpha r^2(\cos(l\pi)+1) = 2r^2\cos(h\pi)(\cos(l\pi)+1) - 4(\cos(l\pi)-1)$$

it can also be written as follows, to get the value of α.

$$\alpha = 2\cos(h\pi) - \frac{4}{r^2}\left[\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right]. \tag{2.25}$$

Substitute the value of α from (2.25), in equation (2.24) and simplify, it gives us the following nine point, three time level novel implicit scheme.

$$\begin{aligned}
-\frac{r^2}{4}\left[u(x+h,t+l)+u(x-h,t+l)\right] + \left[1+\frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]u(x,t+l) \\
= \frac{r^2}{2}\left[u(x+h,t)+u(x-h,t)\right] + \frac{r^2}{4}\left[u(x+h,t-l)+u(x-h,t-l)\right] \\
+ \left[2 - r^2\cos(h\pi) + 2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]u(x,t) \\
- \left[1+\frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]u(x,t-l)
\end{aligned} \tag{2.26}$$

or in another form, we can write it as

$$\begin{aligned}
-\frac{r^2}{4}\left(u_{m+1}^{n+1}+u_{m-1}^{n+1}\right) + \left[1+\frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]u_m^{n+1} \\
= \frac{r^2}{2}\left(u_{m+1}^{n}+u_{m-1}^{n}\right) + \frac{r^2}{4}\left(u_{m+1}^{n-1}+u_{m-1}^{n-1}\right) \\
+ \left[2 - r^2\cos(h\pi) + 2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]u_m^{n} \\
- \left[1+\frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]u_m^{n-1}.
\end{aligned}$$

In the next step, we are going to check the exactness of this novel scheme (2.26). To perform this task, we apply the scheme (2.26) on (mh, nl) node. Now, since we know that $u(x,t) = \sin(\pi x)\cos(\pi t)$, it gives $u(mh,nl) = \sin(mh\pi)\cos(nl\pi)$. Similarly, we can define it for $u((m+1)h,nl)$, $u((m-1)h,nl)$, $u(mh,(n+1)l)$, $u(mh,(n-1)l)$, $u((m+1)h,(n+1)l)$, $u((m+1)h,(n-1)l)$, $u((m-1)h,(n+1)l)$ and $u((m-1)h,(n-1)l)$. The scheme (2.26), when applied at (mh,nl) gives after rearranging

$$\begin{aligned}
&\sin(mh\pi)\cos((n+1)l\pi) - \frac{r^2}{4}\sin((m-1)h\pi)\cos((n+1)l\pi) \\
&+\frac{r^2}{2}\sin(mh\pi)\cos(h\pi)\cos((n+1)l\pi) - \frac{r^2}{4}\sin((m+1)h\pi)\cos((n+1)l\pi) \\
&-\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)(\sin(mh\pi)\cos((n+1)l\pi)) - 2\sin(mh\pi)\cos(nl\pi) \\
&-\frac{r^2}{2}\sin((m-1)h\pi)\cos(nl\pi) + r^2\sin(mh\pi)\cos(h\pi)\cos(nl\pi) \\
&-2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)(\sin(mh\pi)\cos(nl\pi)) + \sin(mh\pi)\cos((n-1)l\pi) \\
&-\frac{r^2}{2}\sin((m+1)h\pi)\cos(nl\pi) - \frac{r^2}{4}\sin((m-1)h\pi)\cos((n-1)l\pi) \\
&+\frac{r^2}{2}\cos(h\pi)\sin(mh\pi)\cos((n-1)l\pi) - \frac{r^2}{4}\sin((m+1)h\pi)\cos((n+1)l\pi) \\
&-\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)(\sin(mh\pi)\cos((n-1)l\pi))
\end{aligned}$$

When we expand the above equation and further simplify it, we will see that the terms will be canceled making $L.H.S = R.H.S = 0$, it proves the exactness of (2.26). Hence, novel implicit scheme (2.26) is dispersion free.

2.2.4.9 Solution at first time step

In order to compute the solution at first time step, we redefine the schemes (2.23) and (2.26), with the help of (2.13), that is

$$\frac{\partial u}{\partial t} = 0.$$

Now, replace the partial derivative with its second order finite difference approximation.

$$\frac{u(x,t+l) - u(x,t-l)}{2l} = 0. \tag{2.27}$$

By using the Taylor's series expansion of $u(x,t+l)$ and $u(x,t-l)$, that is

$$u(x,t+l) = u(x,t) + lu'(x,t) + \frac{l^2}{2!}u''(x,t) + \frac{l^3}{3!}u'''(x,t) + \frac{l^4}{4!}u^4(x,t) + \cdots$$

and

$$u(x,t-l) = u(x,t) - lu'(x,t) + \frac{l^2}{2!}u''(x,t) - \frac{l^3}{3!}u'''(x,t) + \frac{l^4}{4!}u^4(x,t) + \cdots$$

from the above two equations define $u(x,t+l)-u(x,t-l)$, as below

$$u(x,t+l)-u(x,t-l)=2lu'(x,t)+2\frac{l^3}{3!}u'''(x,t)+2\frac{l^5}{5!}u^5(x,t)+\cdots$$

$$u(x,t+l)-u(x,t-l)=2[lu'(x,t)+\frac{l^3}{3!}u'''(x,t)+\frac{l^5}{5!}u^5(x,t)+\cdots] \tag{2.28}$$

Again as $u(x,t)=\sin(\pi x)\cos(\pi t)$. Therefore, we can define the partial derivative with respect to $'t'$ as follows

$$\begin{aligned}
u'(x,t) &= -\pi\sin(\pi x)\sin(\pi t)\\
u''(x,t) &= -\pi^2\sin(\pi x)\cos(\pi t)\\
u'''(x,t) &= \pi^3\pi\sin(\pi x)\sin(\pi t)\\
u^4(x,t) &= \pi^4\sin(\pi x)\cos(\pi t)\cdots.
\end{aligned}$$

From above insert the value of odd order partial derivatives w.r.t $'t'$ in (2.28), we get

$$u(x,t+l)-u(x,t-l)=2\left[-l\pi+\frac{(l\pi)^3}{3!}-\frac{(l\pi)^5}{5!}+\cdots\right]\sin(\pi x)\sin(\pi t)$$

the compact form of above is

$$u(x,t+l)-u(x,t-l)=-2\sin(l\pi)\sin(\pi x)\sin(\pi t). \tag{2.29}$$

We can check the exactness of (2.29), by applying it on (mh,nl) point of the solution, as follows

$$\sin(\pi mh)\cos(\pi(n+1)l)-\sin(\pi mh)\cos(\pi(n-1)l)+2\sin(l\pi)\sin(\pi mh)\sin(\pi nl)=0.$$

After solving the above we get $L.H.S=R.H.S=0$, it means that (2.29) is exact. Now, using (2.29) instead of (2.27), in (2.23), it will give us the scheme for the first time step of explicit system, defined below

$$\begin{aligned}
u_m^{n+1} = (\cos(l\pi)-r^2\cos(h\pi))u_m^n+\frac{r^2}{2}\left(u_{m+1}^n+u_{m-1}^n\right)\\
-\sin(l\pi)\sin(nl\pi)\sin(mh\pi).
\end{aligned}$$

Again, we have to check the exactness of the scheme at first time step and applying it on the node (mh, nl), gives

$$\sin(\pi mh)\cos(\pi(n+1)l) - (\cos(l\pi) - r^2\cos(h\pi))\sin(\pi mh)\cos(\pi nl)$$
$$-\frac{r^2}{2}\left(\sin(\pi(m+1)h)\cos(\pi nl) + \sin(\pi(m-1)h)\cos(\pi nl)\right) + \sin(l\pi)\sin(nl\pi)\sin(mh\pi).$$

Simplify the above equation, we get $L.H.S = R.H.S = 0$, it means that the novel explicit scheme is exact at first time step. Similarly, using (2.29) instead of (2.27), in (2.26), will give us the scheme to compute the solution at first time step of implicit system, defined below

$$\begin{aligned}
-\frac{r^2}{4}\left(u_{m+1}^{n+1} + u_{m-1}^{n+1}\right) + 2\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^{n+1} \\
= \left[2 - r^2\cos(h\pi) + 2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^n \\
+\frac{r^2}{2}\left(u_{m-1}^n + u_{m+1}^n\right) + \frac{r^2}{4}\left(u_{m+1}^{n-1} + u_{m-1}^{n-1}\right) \\
-2\sin(l\pi)\sin(mh\pi)\sin(nl\pi)\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right].
\end{aligned}$$

We now apply the scheme on node (mh, nl), to check the exactness of above scheme, we have

$$\begin{aligned}
-\frac{r^2}{4}\left[\sin(\pi(m+1)h)\cos(\pi(n+1)l) + \sin(\pi(m-1)h)\cos(\pi(n+1)l)\right] \\
+2\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]\sin(\pi mh)\cos(\pi(n+1)l) \\
-\left[2 - r^2\cos(h\pi) + 2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]\sin(\pi mh)\cos(\pi nl) \\
-\frac{r^2}{2}\left[\sin(\pi(m-1)h)\cos(\pi nl) + \sin(\pi(m+1)h)\cos(\pi nl)\right] \\
-\frac{r^2}{4}\left[\sin(\pi(m+1)h)\cos(\pi(n-1)l) + \sin(\pi(m-1)h)\cos(\pi(n-1)l)\right] \\
+2\sin(l\pi)\sin(\pi x)\sin(\pi t)\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right].
\end{aligned}$$

Performing simplifications result into $L.H.S = R.H.S = 0$, which means the novel implicit scheme is exact at first time step.

2.2.4.10 Full system for novel explicit C.F.D scheme

The full system of novel explicit scheme, proposed to solve the first model problem is given as follows.

$$\text{at } m = 0, n = 0, 1, 2, \cdots$$

$$u_m^n = 0,$$

$$\text{at } m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^n = \sin(mh\pi),$$

$$\text{at } m = 1, 2, \ldots, N-1, n = 0$$

$$u_m^{n+1} = [\cos(l\pi) - r^2 \cos(h\pi)]u_m^n + \frac{r^2}{2}\left(u_{m+1}^n + u_{m-1}^n\right)$$

$$- \sin(l\pi)\sin(nl\pi)\sin(mh\pi)$$

$$\text{at } m = 1, 2, \ldots, N-1, n = 1, 2, \cdots$$

$$u_m^{n+1} = 2[\cos(l\pi) - r^2 \cos(h\pi)]u_m^n + r^2(u_{m+1}^n + u_{m-1}^n) - u_m^{n-1}$$

$$\text{at } m = N, n = 0, 1, 2, \cdots$$

$$u_m^n = 0.$$

2.2.4.11 Full system for novel implicit C.F.D scheme

The full system of novel implicit scheme, to solve the first model problem is given below.

$$\text{at } m = 0, n = 0, 1, 2, \cdots$$

$$u_m^n = 0,$$

$$\text{at } m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^n = \sin(mh\pi),$$

$$\text{at } m = 1, 2, \ldots, N-1, n = 0$$

$$\begin{aligned}
-\frac{r^2}{4}\left(u_{m+1}^{n+1} + u_{m-1}^{n+1}\right) + 2\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^{n+1} \\
= \left[2 - r^2\cos(h\pi) + 2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^n \\
+\frac{r^2}{2}\left(u_{m-1}^n + u_{m+1}^n\right) + \frac{r^2}{4}\left(u_{m+1}^{n-1} + u_{m-1}^{n-1}\right) \\
-2\sin(l\pi)\sin(mh\pi)\sin(nl\pi)\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right]
\end{aligned}$$

$$\text{at } m = 1, 2, \cdots, N-1, n = 1, 2, \cdots$$

$$\begin{aligned}
-\frac{r^2}{4}\left(u_{m+1}^{n+1} + u_{m-1}^{n+1}\right) + \left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^{n+1} \\
= \left[2 - r^2\cos(h\pi) + 2\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^n \\
+\frac{r^2}{2}\left(u_{m-1}^n + u_{m+1}^n\right) + \frac{r^2}{4}\left(u_{m+1}^{n-1} + u_{m-1}^{n-1}\right) \\
-\left[1 + \frac{r^2}{2}\cos(h\pi) - \left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\right] u_m^{n-1}
\end{aligned}$$

$$\text{at } m = N, n = 0, 1, 2, \cdots$$

$$u_m^n = 0.$$

2.2.4.12 Combined form of novel explicit and implicit schemes for first model problem

We can write both the novel explicit and implicit schemes for the first model problem in combined form, in the following way. The general form for the first time step is

$$
\begin{aligned}
&-r^2a(u_{m-1}^{n+1}+u_{m+1}^{n+1})+2\left\{1+a\left(2r^2\cos(h\pi)-4\left[\frac{\cos(l\pi)-1}{\cos(l\pi)-1}\right]\right)\right\}u_m^{n+1}\\
&\quad=-r^2(-1+2a)[u_{m-1}^{n}+u_{m+1}^{n}]+\Bigg\{8a+2(-1+3a)r^2\cos(h\pi)\\
&\qquad+2(1-4a)\cos(l\pi)+8a\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\Bigg\}u_m^n\\
&\qquad+r^2a(u_{m-1}^{n-1}+u_{m+1}^{n-1})\\
&\quad-2\sin(l\pi)\sin(\pi x)\sin(\pi t)\left\{1+a\left(2r^2\cos(h\pi)-4\left[\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right]\right)\right\}.
\end{aligned}
$$

Which leads back to the first time step schemes for explicit and implicit system for the values of $a=0$ and $a=1/4$ respectively. Moreover, the combined form for internal nodes as follows.

$$
\begin{aligned}
&-r^2a(u_{m-1}^{n+1}+u_{m+1}^{n+1})+\left\{1+a\left(2r^2\cos(h\pi)-4\left[\frac{\cos(l\pi)-1}{\cos(l\pi)-1}\right]\right)\right\}u_m^{n+1}\\
&\quad=-r^2(-1+2a)[u_{m-1}^{n}+u_{m+1}^{n}]+\Bigg\{8a+2(-1+3a)r^2\cos(h\pi)\\
&\qquad+2(1-4a)\cos(l\pi)+8a\left(\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right)\Bigg\}u_m^n\\
&\quad+r^2a(u_{m-1}^{n-1}+u_{m+1}^{n-1})-\left\{1+a\left(2r^2\cos(h\pi)-4\left[\frac{\cos(l\pi)-1}{\cos(l\pi)+1}\right]\right)\right\}u_m^{n-1}.
\end{aligned}
$$

Which ends up with (2.23) and (2.26), for the values of $a=0$ and $a=1/4$ respectively. This problem has Dirichlet boundary conditions at both ends. So, we do not need to write the general form for the boundary points as we know the value of $u(x,t)$, at the boundary.

2.2.4.13 First problem analysis using standard explicit and implicit schemes and novel explicit and implicit schemes

To show the effectiveness of the novel C.F.D schemes, in this section we consider two types of numerical errors. The first type of error is defined by $Z_m^n = u_m^n - \tilde{U}_m^n$, where u_m^n represents the exact solution of the problem and $\tilde{U}_m^n$ is the numerical solution obtained by using all schemes. The value is computed in between the range $0 \leq x \leq 1$ where the error is greater, and at time $t = 1$. The second type of error we consider is discrete l_∞ norm, defined as

$$E_\infty = max_{m=1,2,\cdots,N} max_{n=1,2,\cdots,} |u_m^n - \tilde{U}_m^n|$$

Scheme	Standard Explicit	Novel Explicit	Standard Implicit	Novel Implicit
Error	$Z,\, E_\infty$	$Z,\, E_\infty$	$Z,\, E_\infty$	$Z,\, E_\infty$
r=0.25	$-0.73 * 10^{-4},\, 0.154679$	$-1.99 * 10^{-15},\, 1.17 * 10^{-13}$	$-0.10 * 10^{-3},\, 0.185388$	$-2.99 * 10^{-15},\, 9.8 * 10^{-13}$
r=0.5	$-0.47 * 10^{-4},\, 0.61 * 10^{-1}$	$-2.22 * 10^{-16},\, 2.43 * 10^{-14}$	$-0.18 * 10^{-3},\, 0.123206$	$-1.33 * 10^{-15},\, 1.74 * 10^{-13}$
r=1	$0,\, 1.09 * 10^{-15}$	$0,\, 1.09 * 10^{-15}$	$-0.72 * 10^{-3},\, 0.121969$	$0,\, 0.7 * 10^{-14}$
r=2	$-0.82 * 10^{-3},\, 6.62 * 10^{-1}$	$1.33 * 10^{-13},\, 2.34 * 10^{-12}$	$-0.59 * 10^{-2},\, 0.177447$	$2.22 * 10^{-16},\, 3.21 * 10^{-15}$
r=5	$-0.99 * 10^{-1},\, 0.323569$	$8.43 * 10^{-14},\, 2.27 * 10^{-13}$	$-0.116021,\, 0.356874$	$-2.22 * 10^{-16},\, 1.32 * 10^{-15}$

Table 2.1: Errors for single mode of vibrating string

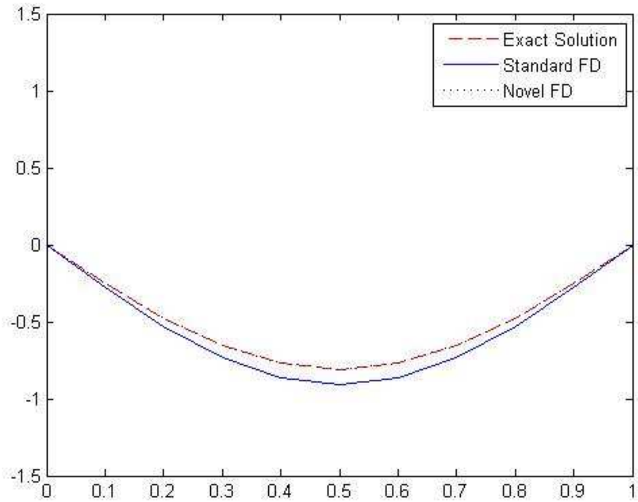

Figure 2.4: Vibrating string with single mode, $h = 0.1$, $l = 0.4$ with E_∞ in standard explicit scheme is 0.8323 and in novel explicit scheme is $1.18 * 10^{-8}$.

In Table 2.1, we compared the performance of standard C.F.D schemes with the novel C.F.D schemes, with single mode, having fixed spatial step size $h = 0.1$ and $r = 0.25, 0.5, 1, 2, 5$, corresponding to time increment $l = 0.025, 0.05, 0.1, 0.2, 0.5$, respectively. From the results, we can clearly observe that the novel schemes provide more accurate results then the standard schemes in all cases, even when r increases. Since, $r = 1$ is a magical number [4], therefore the standard and novel explicit schemes are displaying the same behaviour.

The superiority of the novel schemes is also evident from the figures. Such as, in Figure 2.4, the dispersion in the standard explicit wave is visible, on the other hand the novel wave is the perfect interpolate of the exact wave. Whereas, when $r = 1$ in Figure 2.5 there is no dispersion in any explicit scheme. Next, if we look at the Figure 2.6 and 2.7, in both, even when $r = 1$, the standard implicit wave is showing dispersion in contrast to the novel implicit wave, which is exact.

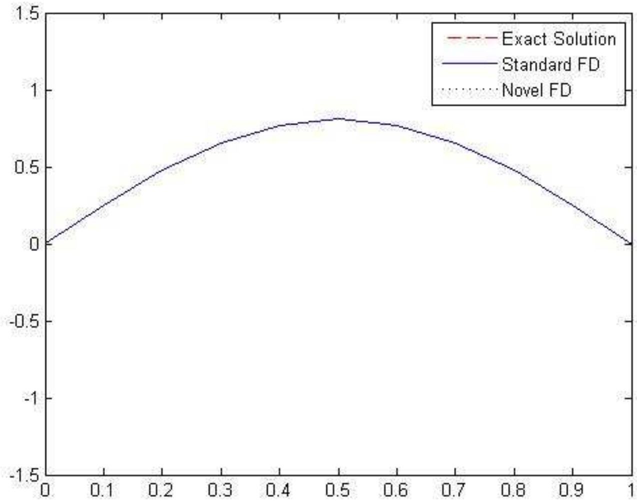

Figure 2.5: Vibrating string with single mode, $h = 0.1$, $l = 0.1$ with E_∞ is same in standard explicit scheme and novel explicit scheme, that is $1.09 * 10^{-15}$.

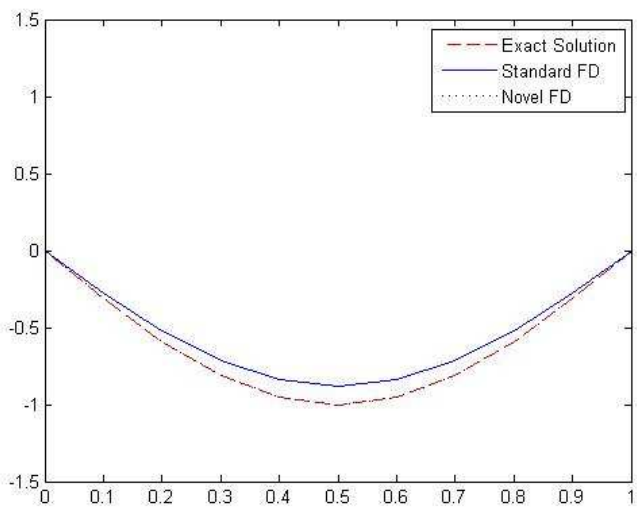

Figure 2.6: Vibrating string with single mode , $h = 0.1$, $l = 0.5$ with E_∞ in standard implicit scheme is 8.2188 and in novel implicit scheme is $1.11 * 10^{-14}$.

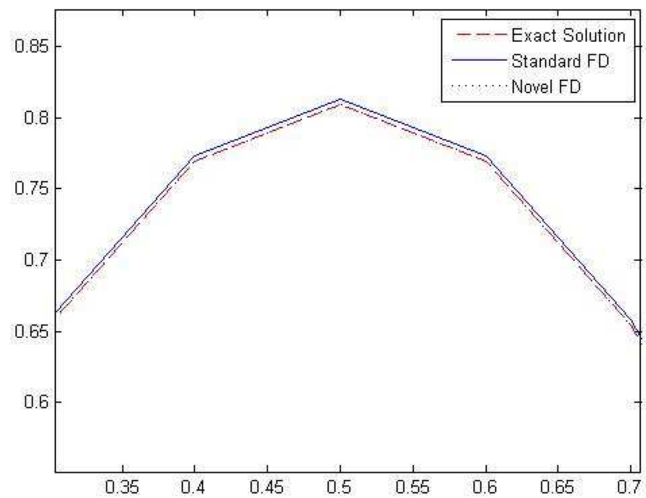

Figure 2.7: Vibrating string with single mode , $h = 0.1$, $l = 0.1$ with E_∞ in standard implicit scheme is 0.4884 and in novel implicit scheme is $2.73 * 10^{-14}$.

If we consider three modes of the vibrating string problem, then we have the following observations.

Scheme	Standard Explicit	Novel Explicit	Standard Implicit	Novel Implicit
Error	Z, E_∞	Z, E_∞	Z, E_∞	Z, E_∞
r=0.25	0.052464, 4.280952	$-3.55 * 10^{-15}$, $1.62 * 10^{-13}$	0.072698, 5.075391	$2.22 * 10^{-15}$, $2.08 * 10^{-13}$
r=0.5	0.034941, 1.743543	$-2.22 * 10^{-16}$, $2.86 * 10^{-15}$	0.120635, 3.327979	$-6.66 * 10^{-16}$, $1.95 * 10^{-14}$
r=1	$-4.44 * 10^{-16}$, $3.65 * 10^{-16}$	$-4.44 * 10^{-16}$, $3.65 * 10^{-16}$	0.379509, 3.073243	$-4.44 * 10^{-16}$, $0.83 * 10^{-15}$
r=2	1.379103, 3.673944	$-7.43 * 10^{-12}$, $1.77 * 10^{-11}$	1.463473, 3.752919	0, $1.83 * 10^{-15}$
r=5	$1.73 * 10^{2}$, $1.82 * 10^{2}$	$8.03 * 10^{-14}$, $4.65 * 10^{-13}$	0.911084, 1.586022	$3.33 * 10^{-16}$, $5.54 * 10^{-15}$

Table 2.2: Errors for three modes of vibrating string

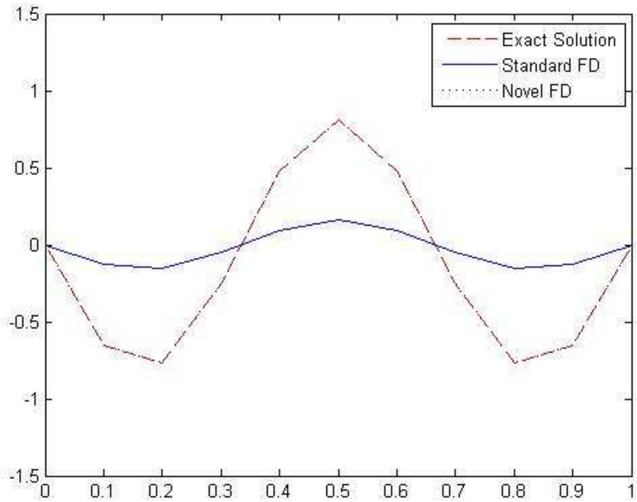

Figure 2.8: Three modes in vibrating string, $h = 0.1$, $l = 0.2$ with E_∞ in standard explicit scheme is 3.6739 and in novel explicit scheme is $1.77 * 10^{-11}$.

In the Table 2.2, we compared the performance of standard C.F.D schemes with the novel C.F.D schemes, with three modes of the string, having fixed spatial step size $h = 0.1$ and $r = 0.25, 0.5, 1, 2, 5$, corresponding to time increment $l = 0.025, 0.05, 0.1, 0.2, 0.5$, respectively. From the results, we can clearly observe that the novel schemes provides more accurate results then the standard schemes in all cases even when r is large. As, $r = 1$, is a magical number [4], so both explicit schemes are showing same behaviour.

When we observe the same vibrating string problem with three modes, in Figure 2.8, again the dispersion in the standard explicit wave is visible. Whereas, when $r = 1$ in Figure 2.9 there is no dispersion in any explicit scheme. Next, if we look at the Figure 2.10 the standard implicit wave is showing dispersion in contrast to the novel implicit wave. Even when $r = 1$ in Figure 2.11, the standard wave is displaying totally useless results by making trough when the exact and novel wave are making trough.

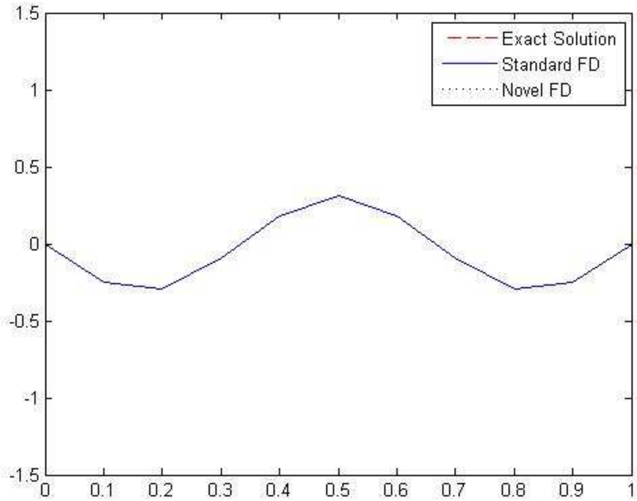

Figure 2.9: Three modes in vibrating string, $h = 0.1$, $l = 0.1$ with E_∞ in standard explicit scheme is $3.65 * 10^{-15}$ and in novel explicit scheme is $3.65 * 10^{-15}$.

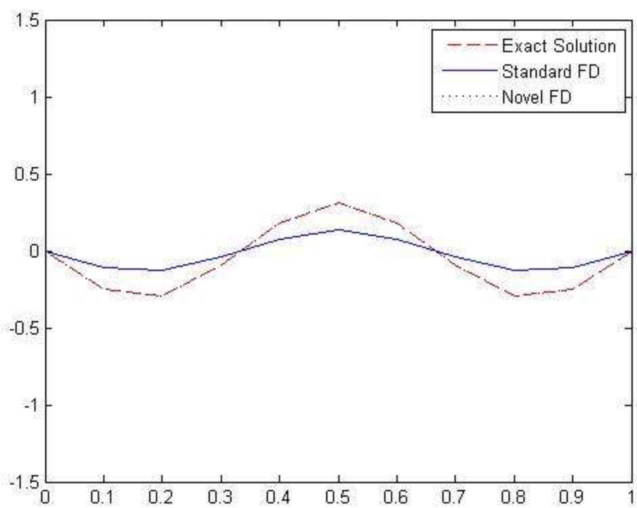

Figure 2.10: Three modes in vibrating string, $h = 0.1$, $l = 0.3$ with E_∞ in standard implicit scheme is 8.9065 and in novel implicit scheme is $2.30 * 10^{-14}$.

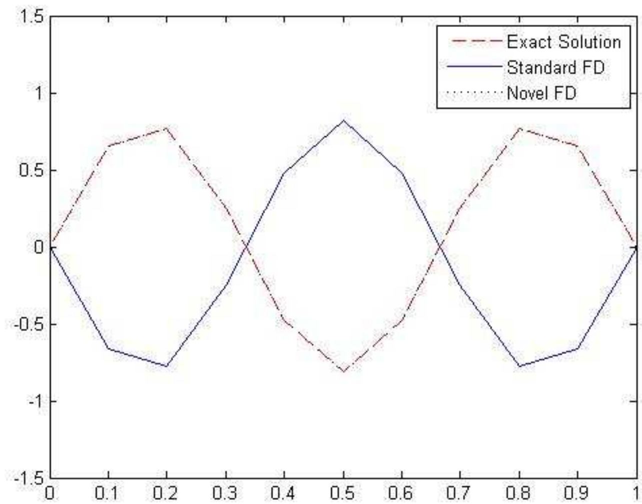

Figure 2.11: Three modes in vibrating string, $h = 0.1$, $l = 0.1$ with E_∞ in standard implicit scheme is 3.07324 and in novel implicit scheme is $6.83 * 10^{-15}$.

2.2.5 Second model problem: wave propagation

Consider the initial boundary value problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \tag{2.30}$$

defined in the (x, t) plane and region $R = [0 < x < 1] * [t > 0]$, with boundary ∂R together with the boundary conditions,

$$u(0,t) = e^{ikt} \text{ and } \frac{\partial u(1,t)}{\partial x} + \frac{\partial u(1,t)}{\partial t} = 0 \quad t > 0 \tag{2.31}$$

and initial conditions

$$u(x,0) = e^{-ikx} \; and \; \frac{\partial u(x,0)}{\partial t} = -ike^{ikx} \quad 0 \le x \le 1. \tag{2.32}$$

The exact solution of this problem is,

$$u(x,t) = e^{ik(x-t)}. \tag{2.33}$$

It is an example of wave propagation, having Dirichlet boundary condition at left end and Robins boundary condition at the right end, with initial displacement

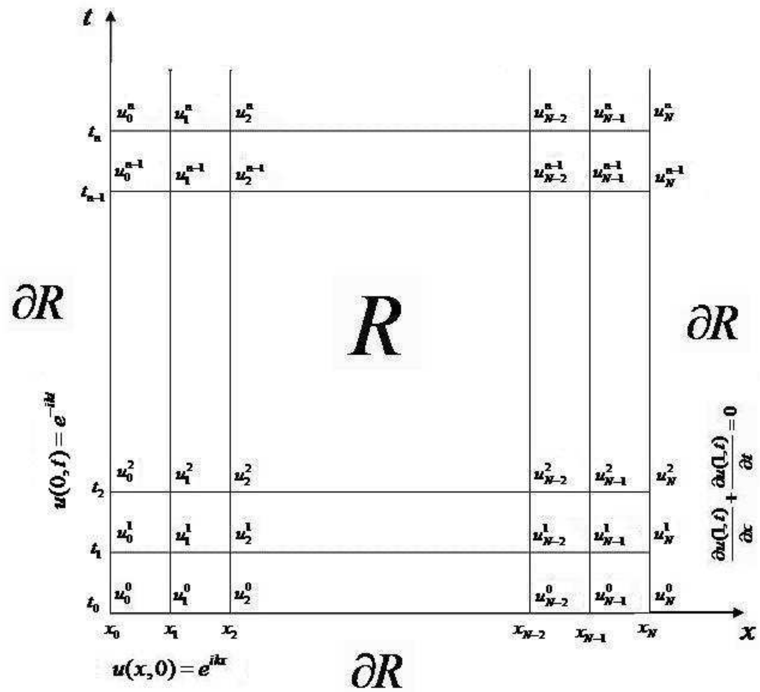

Figure 2.12: Domain of the second problem.

defined by, e^{ikx} and initial velocity given as, $-ike^{ikx}$. Here in this problem the propagation speed is taken as, $c^2 = 1$. The boundary conditions at $x = 0$ (origin) and at $x = 1$ holds for arbitrary t and similarly the initial condition at $t = 0$ holds for $0 \leq x \leq 1$. We can observe clearly the continuity between the initial and the boundary conditions at origin since $u(0, 0) = 0$. We have discretized our domain, the interval $[0, 1]$ is divided into N subintervals each having the constant width, h. So that $h = (b-a)/(N)$ and similarly the time, $t \geq 0$ is divided into equal time steps of length, l. Hence, we can write $x_m = mh$ and $t_n = nl$. Therefore, each node has coordinates of the following form.
$(x_m, t_n) = (mh, nl)$
with $m = 0, 1, 2, \cdots, N$ and $n = 0, 1, 2, \cdots$.
The region R, is an open rectangle bounded by $x = 0$, $x = 1$ and $t = 0$, further it is covered by a grid consist of lines parallel to the time axis (t$-$axis) and the lines parallel to the space axis (x$-$axis).

2.2.5.1 Model problem two: standard second order explicit C.F.D scheme

First of all, we will construct the standard second order central finite difference explicit scheme for the above defined wave propagation problem. Therefore, replace the time partial derivative, $\partial^2 u/\partial t^2$ and the space partial derivative, $\partial^2 u/\partial x^2$ in (2.30) by their second order central finite difference approximations, they are defined in (2.15) and (2.16). This dual replacement is much quicker. After making the substitution in (2.30),

$$\frac{u(x, t+l) - 2u(x, t) + u(x, t-1)}{l^2} = \frac{u(x+h, t) - 2u(x, t) + u(x-h, t)}{h^2}$$

by rearranging, we get

$$u(x, t+l) = 2(1-r^2)u(x, t) + r^2[u(x+h, t) + u(x-h, t)] - u(x, t-1) \quad (2.34)$$

where $r = l/h$, or we can write it as follows

$$u_m^{n+1} = 2(1-r^2)u_m^n + r^2(u_{m+1}^n + u_{m-1}^n) - u_m^{n-1}.$$

2.2.5.2 Solution at last node

The above scheme can be used for the computation of internal nodes only, because as we apply this scheme at the Nth node it gives us the fictitious node, also known as fantom node, this lies outside our boundary and we have no information about the value of this node. Therefore, there is a need to remove it, thus we redefine (2.34) for last node with the help of non−reflecting boundary condition at right end.

Consider the non −reflecting boundary condition from (2.31), that is

$$\frac{\partial u(x,t)}{\partial x} + \frac{\partial u(x,t)}{\partial t} = 0. \tag{2.35}$$

Replace $\partial u(x,t)/\partial x$ and $\partial u(x,t)/\partial t$ by their second order finite difference approximation, that is

$$\frac{\partial u(x,t)}{\partial x} = \frac{1}{2h}\left[u(x+h,t) - u(x-h,t)\right] + O(h^2), \tag{2.36}$$

and

$$\frac{\partial u(x,t)}{\partial t} = \frac{1}{2l}\left[u(x,t+l) - u(x,t-l)\right] + O(l^2). \tag{2.37}$$

By using (2.36) and (2.37) in (2.35), we get the following after rearranging the terms.

$$r[u(x+h,t) - u(x-h,t)] + [u(x,t+l) - u(x,t-l)] = 0$$

further we can say that,

$$u(x+h,t) = u(x-h,t) - \frac{1}{r}\left[u(x,t+l) - u(x,t-l)\right]. \tag{2.38}$$

Insert the value of $u(x+h,t)$ from (2.38) in (2.34), and after further simplification we have the required scheme for last node as below,

$$u(x,t+l) = 2(1-r)u(x,t) + \frac{2r^2}{1+r}u(x-h,t) - \frac{1-r}{1+r}u(x,t-1) \tag{2.39}$$

or we can write it as,

$$u_m^{n+1} = 2(1-r)u_m^n + \frac{2r^2}{1+r}u_{m-1}^n - \frac{1-r}{1+r}u_m^{n-1}.$$

2.2.5.3 Solution at first time step

This subsection has the purpose to calculate the value of $u(x,t)$, at the first time step. Since, it is not explicitly contained in the initial conditions. Therefore, we need a sufficiently accurate approximation to the dependent variable at the first time step, to be used in (2.34). Here, we make use of initial velocity given in (2.32), that is

$$\frac{\partial u}{\partial t} = -iku(x,t),$$

Now, replace the partial derivative with its second order finite difference approximation.

$$\frac{u(x,t+l) - u(x,t-l)}{2l} = -iku(x,t)$$

$$u(x,t-l) = u(x,t+l) + 2ilku(x,t). \tag{2.40}$$

Using (2.40) in (2.34), we get the following scheme to compute solution at first time step of explicit system.

$$u_m^{n+1} = (1 - r^2 - ilk)u_m^n + \frac{r^2}{2}\left(u_{m+1}^n + u_{m-1}^n\right).$$

2.2.5.4 Full system for standard explicit C.F.D scheme

The full system for the second model problem is given below.

$$\text{at } m = 0, n = 0, 1, 2 \cdots$$

$$u_m^n = e^{-inlk},$$

$$\text{at } m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^n = e^{imhk},$$

$$\text{at } m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^{n+1} = (1 - r^2 - ilk)u_m^n + \frac{r^2}{2}\left(u_{m+1}^n + u_{m-1}^n\right)$$

$$\text{at } m = 1, 2, \cdots, N-1, n = 1, 2, \cdots$$

$$u_m^{n+1} = 2(1 - r^2)u_m^n + r^2(u_{m+1}^n + u_{m-1}^n) - u_m^{n-1}$$

$$\text{at } m = N, n = 0, 1, 2, \cdots$$

$$u_m^{n+1} = 2(1 - r)u_m^n + \frac{2r^2}{1+r}u_{m-1}^n - \frac{1-r}{1+r}u_m^{n-1}.$$

2.2.5.5 Construction of novel explicit C.F.D scheme for model problem two

In this section we will construct novel explicit C.F.D scheme for the wave propagation problem. Reconsider it, and this time we replace the partial derivatives $\partial^2 u/\partial x^2$ and $\partial^2 u/\partial t^2$ by the following.

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

and

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{l^2}\left[u(x,t+l) - \alpha u(x,t) + u(x,t-l)\right] + O(l^2).$$

Here, the standard C.F.D approximations for spatial as well as the temporal part are modified by assigning α as a weight of the central node, instead of 2. After using these substitutions in the equation (2.30), we have the form.

$$[u(x,t+l) - \alpha u(x,t) + u(x,t-l)] = r^2[u(x+h,t) - \alpha u(x,t) + u(x-h,t)] \quad (2.41)$$

where $r = l/h$.

As here α is unknown, so the second step is to find the value of this α. Therefore, consider the exact solution $u(x,t) = e^{ik(x-t)}$, and define the following,

$$\begin{aligned} u(x+h,t) &= e^{ik(x+h-t)} \\ u(x-h,t) &= e^{ik(x-h-t)} \\ u(x,t+l) &= e^{ik(x-t-l)} \\ \text{and} \quad u(x,t-l) &= e^{ik(x-t+l)}. \end{aligned}$$

Using these substitutions in (2.41), we have

$$e^{ik(x-t-l)} - \alpha e^{ik(x-t)} + e^{ik(x-t+l)} = r^2[e^{ik(x+h-t)} - \alpha e^{ik(x-t)} + e^{ik(x-h-t)}]$$

after simplifying we are left with,

$$\begin{aligned} [2r^2\cos(hk) + \alpha(1-r^2) - 2\cos(lk)]e^{ik(x-t)} &= 0 \\ \text{or} \quad [2r^2\cos(hk) + \alpha(1-r^2) - 2\cos(lk)]u(x,t) &= 0. \end{aligned}$$

Since, we know that $u(x,t) \neq 0$. It means,

$$2r^2\cos(hk) + \alpha(1 - r^2) - 2\cos(lk) = 0$$

rearranging the above expression to get the value of α.

$$\alpha = \frac{2}{1 - r^2}\left(\cos(lk) - r^2\cos(hk)\right). \tag{2.42}$$

Insert the value of α from (2.42), in equation (2.41) and simplify, it gives us the following five point, two time level novel explicit scheme.

$$u(x,t+l) = 2[\cos(lk) - r^2\cos(hk)]u(x,t) + r^2[u(x-h,t) + u(x+h,t)] - u(x,t-l) \tag{2.43}$$

or in another form, we can write it as

$$u_m^{n+1} = 2[\cos(lk) - r^2\cos(hk)]u_m^n + r^2[u_{m-1}^n + u_{m+1}^n] - u_m^{n-1}.$$

In the next step, we are going to check the exactness of this, (2.43) novel explicit scheme. In order to do so, we apply the scheme, (2.43) on (mh, nl) node. Now, since we know that $u(x,t) = e^{ik(x-t)}$, so it gives $u(mh, nl) = e^{ik(mh-nl)}$. Similarly, we can define it for $u((m+1)h, nl)$, $u((m-1)h, nl)$, $u(mh, (n+1)l)$ and $u(mh, (n-1)l)$. The scheme, (2.43) when applied at (mh, nl) gives after rearranging

$$e^{ik(mh-nl-l)} - 2(\cos(lk) - r^2\cos(hk))e^{ik(mh-nl)}$$
$$-r^2(e^{ik(mh+h-nl)} + e^{ik(mh-h-nl)}) + e^{ik(mh-nl+l)} = 0$$

All the terms will be canceled making $L.H.S = R.H.S = 0$, it proves the exactness of (2.43). Hence, (2.43) is dispersion free.

2.2.5.6 Solution at last node

When the scheme (2.43) is used for the computation of Nth node value it gives us the fictitious node. So, we need to remove it by using the given non−reflecting boundary condition at right end. Now this time again it is not as easier task to make this non−reflecting boundary condition exact, since it involves the spatial as well as the temporal first order partial derivatives, we have to make the dual replacement.

Thus, consider the non −reflecting boundary condition from (2.31), and replace $\partial u/\partial x$ and $\partial u/\partial t$ by their second order finite difference approximation, defined in (2.36) and (2.37), which gives us the following form

$$\frac{1}{2h}\left[u(x+h,t)-u(x-h,t)\right]+\frac{1}{2l}\left[u(x,t+l)-u(x,t-l)\right]=0$$

or it can be written as,

$$\frac{1}{h}\left[u(x+h,t)-u(x-h,t)\right]+\frac{1}{l}\left[u(x,t+l)-u(x,t-l)\right]=0 \tag{2.44}$$

Since, we know by the Taylor's series expansion of $u(x+h,t)$ and $u(x-h,t)$, that

$$u(x+h,t)=u(x,t)+hu'(x,t)+\frac{h^2}{2!}u''(x,t)+\frac{h^3}{3!}u'''(x,t)+\frac{h^4}{4!}u^4(x,t)+\cdots$$

and

$$u(x-h,t)=u(x,t)-hu'(x,t)+\frac{h^2}{2!}u''(x,t)-\frac{h^3}{3!}u'''(x,t)+\frac{h^4}{4!}u^4(x,t)+\cdots$$

from the above two equations define $u(x+h,t)-u(x-h,t)$, as below

$$u(x+h,t)-u(x-h,t)=2hu'(x,t)+2\frac{h^3}{3!}u'''(x,t)+2\frac{h^5}{5!}u^5(x,t)+\cdots$$

$$u(x+h,t)-u(x-h,t)=2[hu'(x,t)+\frac{h^3}{3!}u'''(x,t)+\frac{h^5}{5!}u^5(x,t)+\cdots] \tag{2.45}$$

As $u(x,t) = e^{ik(x-t)}$, so define the nth partial derivative with respect to $'x'$ as follows

$$\begin{aligned} u'(x,t) &= iku(x,t) \\ u''(x,t) &= -k^2u(x,t) \\ u'''(x,t) &= -ik^3u(x,t) \\ u^4(x,t) &= k^4u(x,t) \\ . &= . \\ . &= . \\ . &= . \\ u^n(x,t) &= (-1)^{n+1}(ik)^nu(x,t) \text{ where } n = 1,2,3,\cdots. \end{aligned}$$

From above, insert the values of odd order partial derivatives w.r.t $'x'$ in (2.45), we get

$$u(x+h,t) - u(x-h,t) = 2[ihku(x,t) - \frac{i(hk)^3}{3!}u(x,t) + \frac{i(hk)^5}{5!}u(x,t) - \cdots]$$
$$u(x+h,t) - u(x-h,t) = 2i\left[hk - \frac{(hk)^3}{3!} + \frac{(hk)^5}{5!} - \cdots\right]u(x,t)$$

the compact form of above is

$$u(x+h,t) - u(x-h,t) = 2i\sin(hk)u(x,t). \tag{2.46}$$

Similarly, by using the Taylor's series expansion of $u(x,t+l)$ and $u(x,t-l)$, that is

$$u(x,t+l) = u(x,t) + lu'(x,t) + \frac{l^2}{2!}u''(x,t) + \frac{l^3}{3!}u'''(x,t) + \frac{l^4}{4!}u^4(x,t) + \cdots$$

and

$$u(x,t-l) = u(x,t) - lu'(x,t) + \frac{l^2}{2!}u''(x,t) - \frac{l^3}{3!}u'''(x,t) + \frac{l^4}{4!}u^4(x,t) + \cdots$$

from the above two equation define $u(x,t+l) - u(x,t-l)$, as below

$$u(x,t+l) - u(x,t-l) = 2lu'(x,t) + 2\frac{l^3}{3!}u'''(x,t) + 2\frac{l^5}{5!}u^5(x,t) + \cdots$$

$$u(x,t+l) - u(x,t-l) = 2[lu'(x,t) + \frac{l^3}{3!}u'''(x,t) + \frac{l^5}{5!}u^5(x,t) + \cdots] \qquad (2.47)$$

Again as $u(x,t) = e^{ik(x-t)}$, so we can define the nth partial derivative with respect to $'t'$ as follows

$$\begin{aligned}
u'(x,t) &= -iku(x,t) \\
u''(x,t) &= -k^2u(x,t) \\
u'''(x,t) &= ik^3u(x,t) \\
u^4(x,t) &= k^4u(x,t) \\
. &= . \\
. &= . \\
. &= . \\
u^n(x,t) &= (-ik)^n u(x,t) \text{ where } n = 1,2,3,\cdots.
\end{aligned}$$

From above insert the values of odd order partial derivatives w.r.t $'t'$ in (2.47), we get

$$u(x,t+l) - u(x,t-l) = 2[-ilku(x,t) + \frac{i(lk)^3}{3!}u(x,t) - \frac{i(lk)^5}{5!}u(x,t) + \cdots]$$
$$u(x,t+l) - u(x,t-l) = -2i\left[lk - \frac{(lk)^3}{3!} + \frac{(lk)^5}{5!} - \cdots\right]u(x,t)$$

the compact form of above is

$$u(x,t+l) - u(x,t-l) = -2i\sin(lk)u(x,t). \qquad (2.48)$$

Finally, we use (2.46) and (2.48) in (2.44), which gives the following form of the exact non−reflecting boundary condition.

$$u(x+h,t) - u(x-h,t) - 2i\sin(hk)u(x,t)$$
$$+u(x,t+l) - u(x,t-l) + 2i\sin(lk)u(x,t) = 0.$$

by rearranging we can write it as,

$$u(x+h,t) = u(x-h,t) + 2i(\sin(hk) - \sin(lk))u(x,t)$$

$$+[u(x,t-l)-u(x,t+l)]. \tag{2.49}$$

Now, before making use of the value, $u(x+h,t)$, we prove that (2.49) is exact. To perform this task we apply the scheme, (2.49) on (mh, nl) node. Now, since we know that $u(x,t)=e^{ik(x-t)}$, it gives $u(mh,nl)=e^{ik(mh-nl)}$. Similarly, we can define it for $u((m+1)h,nl)$, $u((m-1)h,nl)$, $u(mh,(n+1)l)$ and $u(mh,(n-1)l)$. The scheme, (2.49) when applied at (mh, nl) gives after rearranging

$$\begin{aligned}
e^{ik(mh+h-nl)} - e^{ik(mh-h-nl)} - 2i(\sin(hk)-\sin(lk))e^{ik(mh-nl)}& \\
-e^{ik(mh-nl+l)} + e^{ik(mh-nl-l)}) &= 0
\end{aligned}$$

All the terms will be canceled making $L.H.S = R.H.S = 0$, it proves the exactness of (2.49). So finally, we inset the value of $u(x+h,t)$ from (2.49) into (2.43) and further simplify it to get the following scheme for last node.

$$\begin{aligned}
u(x,t+l) = {}& \frac{2}{(1+r^2)}\left[\cos(lk)+ir^2\sin(hk)-ir^2\sin(lk)-r^2\cos(hk)\right]u(x,t) \\
&+\left(\frac{2r^2}{1+r^2}\right)u(x-h,t)-\left(\frac{1-r^2}{1+r^2}\right)u(x,t-1)
\end{aligned} \tag{2.50}$$

or we can write it as,

$$\begin{aligned}
u_m^{n+1} = {}& \frac{2}{(1+r^2)}\left[\cos(lk)+ir^2\sin(hk)-ir^2\sin(lk)-r^2\cos(hk)\right]u_m^n \\
&+\left(\frac{2r^2}{1+r^2}\right)u_{m-1}^n-\left(\frac{1-r^2}{1+r^2}\right)u_m^{n-1}.
\end{aligned}$$

The exactness of scheme (2.50), is proved below. For this task apply (2.50) on (mh, nl) node. Now, since we know that $u(x,t)=e^{ik(x-t)}$, it gives $u(mh,nl)=e^{ik(mh-nl)}$. Similarly, we can define it for $u((m+1)h,nl)$, $u((m-1)h,nl)$, $u(mh,(n+1)l)$ and $u(mh,(n-1)l)$. The scheme, (2.50) when applied at (mh, nl) gives after rearranging

$$\begin{aligned}
e^{ik(mh-nl-l)} - {}& \frac{2}{(1+r^2)}\left[\cos(lk)+ir^2\sin(hk)-ir^2\sin(lk)-r^2\cos(hk)\right]e^{ik(mh-nl)} \\
&-\left(\frac{2r^2}{1+r^2}\right)e^{ik(mh-h-nl)}+\left(\frac{1-r^2}{1+r^2}\right)e^{ik(mh-nl+l)} = 0
\end{aligned}$$

All the terms will be canceled making $L.H.S = R.H.S = 0$, it proves the exactness of (2.49), and also completes the procedure for the construction of the optimal explicit C.F.D scheme.

2.2.5.7 Solution at first time step

In order to compute the solution at first time step, we redefine the scheme (2.43), with the help of (2.13), that is

$$\frac{\partial u}{\partial t} = -iku(x,t).$$

its exact form is defined as,

$$u(x,t+l) - u(x,t-l) = -2i\sin(lk)u(x,t)$$

or we can write it as,

$$u(x,t-l) = u(x,t+l) + 2i\sin(lk)u(x,t). \tag{2.51}$$

Before using it we prove that it is exact, so apply (2.51) on (mh, nl) node, we get the following equation.

$$e^{ik(mh-nl+l)} - e^{ik(mh-nl-l)} - 2i\sin(lk)e^{ik(mh-nl)} = 0.$$

simplify the above equation, we will get $L.H.S = R.H.S = 0$, this proves the exactness of (2.51). Now, using (2.51) in (2.43), we get the following explicit scheme for the for time step of explicit system.

$$u_m^{n+1} = [\cos(lk) - r^2\cos(hk) - i\sin(lk)]u_m^n + \frac{r^2}{2}[u_{m+1}^n + u_{m-1}^n].$$

Next, we prove its exactness, apply it on (mh, nl) node, we get the following form

$$\begin{aligned} e^{ik(mh-nl-l)} - [\cos(lk) - r^2\cos(hk) - i\sin(lk)] - e^{ik(mh-nl)} \\ -\frac{r^2}{2}[e^{ik(mh+h-nl)} + e^{ik(mh-h-nl)}] = 0. \end{aligned}$$

The simplification of the above equation results into $L.H.S = R.H.S = 0$.

2.2.5.8 Full system of novel explicit C.F.D scheme

The complete explicit system to solve the wave propagation problem is given below

$$\text{at } \; m = 0, n = 0, 1, 2 \cdots$$

$$u_m^n = e^{-inlk},$$

$$\text{at } \; m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^n = e^{-imhk},$$

$$\text{at } \; m = 1, 2, \cdots, N-1, n = 0$$

$$u_m^{n+1} = [\cos(lk) - r^2 \cos(hk) - i\sin(lk)]u_m^n + \frac{r^2}{2}[u_{m+1}^n + u_{m-1}^n]$$

$$\text{at } \; m = 1, 2, \ldots, N-1, n = 1, 2, \cdots$$

$$u_m^{n+1} = 2[\cos(lk) - r^2 \cos(hk)]u_m^n + r^2(u_{m+1}^n + u_{m-1}^n) - u_m^{n-1}$$

$$\text{at } \; m = N, n = 0, 1, 2, \cdots$$

$$\begin{aligned} u_m^{n+1} = & \frac{2}{(1+r^2)}\left[\cos(lk) - r^2 i\sin(lk) + ir^2\sin(hk) - r^2\cos(hk)\right] u_m^n \\ & + \frac{2r^2}{1+r^2}u_{m-1}^n - \frac{1-r^2}{1+r^2}u_m^{n-1}. \end{aligned}$$

2.2.5.9 Second problem analysis using standard explicit and novel explicit schemes

To show the effectiveness of the novel C.F.D scheme, in this section we are going to calculate discrete l_∞ norm, defined as

$$E_\infty = max_{m=1,2,\cdots,N} max_{n=1,2,\cdots,}|u_m^n - \tilde{U}_m^n|.$$

In Table 2.3, we have used $r = 0.05$, and k varies. It is clearly visible that at very very high wave number that is,$k = 10^{10}$ we are getting 10^{-5} accuracy with novel explicit C.F.D scheme. Whereas the standard scheme is showing totaly useless results, it gives not even a single digit accuracy.

In Table 2.4, we have used $r = 0.5$, $h = 0.1$ and k varies. Again as r increases we have good results in case of novel C.F.D scheme, in comparison to the standard scheme.

In Table 2.5, we have used $r = 1$, $h = 0.01$ and k varies. Similarly, We are getting 10^{-5} accuracy at very very high wave number, on the contrary the same accuracy is obtained with standard scheme when the wave number is very very small.

k	Standard Explicit E_∞	Novel Explicit E_∞
10^{10}	$6.21 * 10^{10}$	$3.55 * 10^{-5}$
10^{8}	$7.35 * 10^{8}$	$3.42 * 10^{-7}$
10^{6}	$9.03 * 10^{6}$	$3.51 * 10^{-9}$
10^{4}	$3.85 * 10^{4}$	$3.50 * 10^{-11}$
10^{2}	$6.95 * 10^{2}$	$3.90 * 10^{-13}$
10^{0}	1.8158	$1.95 * 10^{-11}$
10^{-2}	$4.5 * 10^{-3}$	$9.9 * 10^{-12}$
10^{-4}	$4.52 * 10^{-5}$	$2.02 * 10^{-11}$

Table 2.3: Errors by using $r = 0.05$

k	Standard Explicit E_∞	Novel Explicit E_∞
10^{10}	$1.27 * 10^{10}$	$6.28 * 10^{-3}$
10^{8}	$2.16 * 10^{7}$	$2.22 * 10^{-7}$
10^{6}	$1.97 * 10^{5}$	$1.98 * 10^{-9}$
10^{4}	$9.98 * 10^{3}$	$2.32 * 10^{-9}$
10^{2}	$2.89 * 10^{1}$	$1.72 * 10^{-13}$
10^{0}	0.7005	$2.37 * 10^{-14}$
10^{-2}	$7.06 * 10^{-3}$	$2.62 * 10^{-14}$
10^{-4}	$7.06 * 10^{-5}$	$5.32 * 10^{-15}$

Table 2.4: Errors by using $r = 0.5$

k	Standard Explicit E_∞	Novel Explicit E_∞
10^{10}	$1 * 10^{10}$	$6.66 * 10^{-5}$
10^{8}	$9.99 * 10^{7}$	$6.51 * 10^{-7}$
10^{6}	$9.99 * 10^{5}$	$6.67 * 10^{-9}$
10^{4}	$9.99 * 10^{3}$	$6.71 * 10^{-11}$
10^{2}	$1 * 10^{2}$	$6.49 * 10^{-13}$
10^{0}	0.9999	$7.72 * 10^{-15}$
10^{-2}	$1 * 10^{-2}$	$6.49 * 10^{-17}$
10^{-4}	$9.99 * 10^{-5}$	$0.78 * 10^{-19}$

Table 2.5: Errors by using $r = 1$

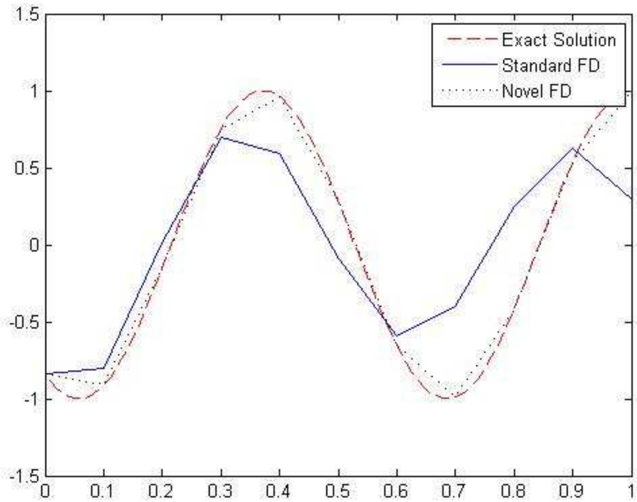

Figure 2.13: Wave propagation, with $h = 0.1$, $l = 0.05$, $k = 10$ and E_∞ in standard is 32.50 and in novel is $6.66 * 10^{-12}$.

In Figure 2.13, the wave number is very moderate, still the standard wave is showing dispersion. Whereas, the novel wave is the perfect interpolate of the exact wave. In Figure 2.14, as the wave number increases to 50, the standard wave is displaying useless results. When the wave number reaches to 100, in Figure 2.15, the standard wave is not even propagating, it has dissipated. On the other hand the novel wave is still the perfect interpolate of the exact wave.

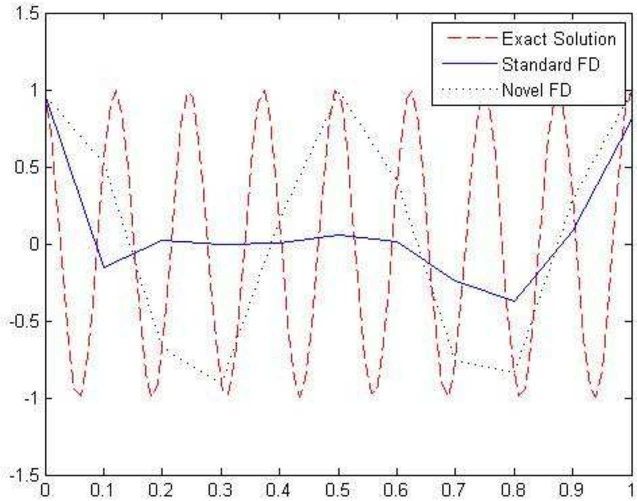

Figure 2.14: Wave propagation, with $h = 0.1$, $l = 0.05$, $k = 50$ and E_∞ in standard is 14.5921 and in novel is $3.69 * 10^{-14}$.

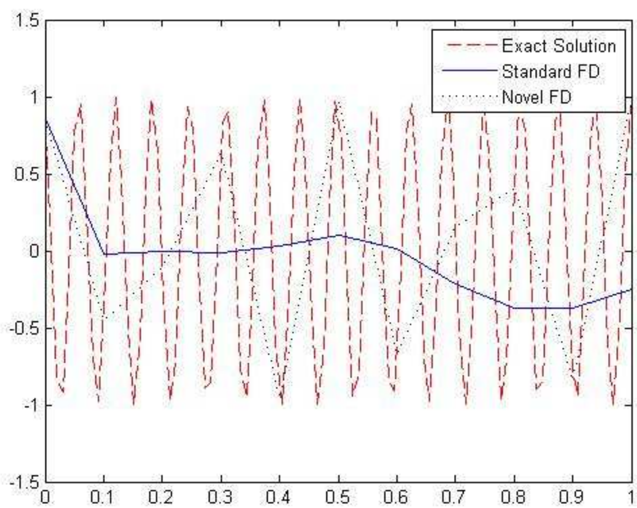

Figure 2.15: Wave propagation, with $h = 0.1$, $l = 0.01$, $k = 100$ and E_∞ in standard is $1.34 * 10^2$ and in novel is $9.78 * 10^{-13}$.

Chapter 3
Conclusions

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Conclusions

Novel explicit and implicit C.F.D schemes, for solving the one dimensional transient wave equation, with rectangular grid, are presented in this work. It is shown that the novel discrete schemes are dispersion free. Since, the idea is very simple, its implementation is quite easy and less costly. The most attractive feature of these novel schemes is that they work for low as well as high wave numbers, without the common requirement of using fine mesh size. One can also recover the standard schemes, as the novel schemes represent the general form. To demonstrate the effectiveness of the novel schemes constructed here, we implemented the idea on vibrating string problem and wave propagation problem. The proofs are given, showing that the novel schemes exactly satisfy the governing partial differential equation, as well as the non−reflecting boundary condition involved in the second problem. Numerical simulations are added to view the effect of the novel schemes, in two ways, with the help of tables. The first purpose is to compare the accuracy, one obtains with the novel schemes, and the second purpose is to observe the computational savings, that one enjoys by using novel schemes, in contrast with the standard schemes. Graphical representations also tell us the same success story.
In the future work, one can extend the idea on some more complicated models, or even on higher dimensions.

Chapter 4
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