An Efficient Finite Difference Discretization for Time-Dependent Multi-Dimensional Partial Differential Equations

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Abstract

Finite difference techniques are widely used for the numerical simulation of time-dependent partial differential equations. In order to get better accuracy at low computational cost, researchers have attempted to develop higher order methods by improving other lower order methods. However, these types of methods usually suffer from a high degree of numerical dispersion. In this thesis, we review three higher order finite difference methods, higher order compact (HOC), compact Padé based (CPD) and non-compact Padé based (NCPD) schemes for the acoustic wave equation. We present the stability analysis of the three schemes and derive dispersion characteristics for these schemes analytically. The effects of Courant–Friedrichs–Lewy (CFL) number, propagation angle and number of cells per wavelength on dispersion are studied.

Declaration

I, the undersigned, hereby declare that the work contained in this research project is my original work, and that any work done by others or by myself previously has been acknowledged and referenced accordingly.

Yahya Ali Abdulkadir, 22 May 2014

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1. Introduction

Real life situations in many disciplines including engineering, physics, economics, biosciences, etc, can be described through mathematical models. Differential equations play an important role in modelling interactions in physics, engineering, and biological processes, from ground motion (earthquake) to interactions between neurons. Differential equations can either be categorized as ordinary differential equations (ODEs), which are for example, used to model dynamical systems and their applications to science and engineering or partial differential equations (PDEs), which most importantly used to describe a wide variety of phenomena in physics; such as sound, heat, fluid dynamics, elasticity and in most field of engineering in general. However, most differential equations, such used to solve real-life problems, have no analytical solutions or are unrealistic to solve analytically. Therefore, solutions for these problems are attempted by means of numerical approximations. To this end various numerical methods are developed to provide better approximate solutions to these equations.

Numerical techniques are a powerful tool for handling large systems of equations involving complex geometries that are otherwise impossible to handle analytically (Canale and Chapra, 1998). There are several types of numerical methods, each with their own pros and cons. Finite difference method (FDM) is the most popular numerical technique which is used to approximate solutions to differential equations using finite difference equations (Zhou, 2013). These techniques are widely used for the numerical solutions of time-dependent partial differential equations. However, when we approximate derivatives using finite difference methods truncation of terms produces inaccuracies. Due to these truncations an inherent problem arises; undesirable ripples are produced due in the process of discretization. Sometimes, due to truncation of higher order terms, frequency dependent numerical errors called dispersion is produced. A large amount of work has been developed for higher order accurate scheme with low dispersion; for instance, Krumpholz and Katehi (1996) developed time-domain schemes based on multiresolution analysis, Tae-Woo and Hagness (2004) introduced a low-dispersive schemes based on Pseudo-spectral approach.

The aim of this research is to explore a higher order compact finite difference scheme with comparably low dispersive characteristics. Therefore, in this paper ,firstly, we will discuss a conventional higher order finite difference schemes .Then we will discuss another higher order finite difference scheme developed by Das et al. (2013) and Liao (2013). We will also discus the dispersion properties of these methods by comparing with a conventional higher order finite difference scheme.

The rest of this thesis is organized as follows: Description of some multi-dimensional time dependent partial differential equations along with initial and boundary values are presented in chapter two. We then descritize the acoustic wave equation for two and three dimensions using Taylor and Padé approximation in chapter three, followed by discussions of higher order finite difference schemes for the stated equation in chapter four. Dispersions and stability analysis for different schemes are shown in chapter five. Finally, discussions of dispersion analysis and comparisons of different higher order schemes are presented in chapter six and conclusions are presented in the last chapter.

2. Multi-Dimensional Time-Dependent Partial Differential Equations (M-D TDPDEs)

Most of the important classes of PDEs in the physical sciences are time-dependent.Therefore, in this chapter we will discuss different types of single and multi-dimensional time dependent partial differential equations.

2.1 The advection equation

The advection (convection) equation is a mathematical equation which is mostly encountered in models of convection of fluids. The advection equation in one dimension is written as (Bradie, 2006)

$$\frac{\partial u}{\partial t} + a(x,t,u)\frac{\partial u}{\partial x} = g(x,t,u). \tag{2.1.1}$$

The boundary and initial conditions are

$$u(x,0) = f(x), \quad 0 < x \leq L, \tag{2.1.2}$$
$$u(0,t) = g_0(t), \tag{2.1.3}$$
$$u(L,t) = g_1(t), \tag{2.1.4}$$
$$u_t(x,0) = g_2(x). \tag{2.1.5}$$

The convection-diffusion equation is written as (Thongmoon et al., 2007)

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_h\frac{\partial^2 C}{\partial x^2} + D_h\frac{\partial^2 C}{\partial y^2} + D_v\frac{\partial^2 C}{\partial z^2}, \tag{2.1.6}$$

with initial and boundary conditions

$$\begin{aligned}
C(x,y,z,0) &= 0, \quad 0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1,\\
C(0,y,z,t) &= 0, \quad 0.5 \leq y \leq 1; 0 \leq z \leq 1,\\
C(1,y,z,0) &= 0, \quad 0 \leq y \leq 1; 0 \leq z \leq 1,\\
\frac{\partial C}{\partial y} &= 0 \quad \text{on} \quad y = 0,1; t > 0,\\
\frac{\partial C}{\partial z} &= 0 \quad \text{on} \quad z = 0,1; t > 0,
\end{aligned} \tag{2.1.7}$$

where $C(x,y,z,t)$ is concentration (mass per unit volume) at point (x,y,z) in Cartesian coordinates and at time t, with speed u, D_h and D_v are constant dispersion coefficients in the horizontal and vertical directions, respectively.

As the name indicates, the convection–diffusion equation is a combination of two equations; the diffusion equation and convection equation. This equation mostly describes physical phenomena in a system due to convection and diffusion processes.

Many authors have discussed the numerical solutions of the advection-diffusion problem. For instance, Mittal and Jain (2012) have discussed a numerical solution for the one-dimensional convection-diffusion equation, Appadu and Gidey (2013) have discussed procedures for time splitting in the 2D advection-diffusion equation, and Shukla et al. (2011) have presented a short survey of numerical methods for solving convection-diffusion problems.

2.2 The diffusion equation

One of the important equation governing heat and mass transfer is the diffusion equation. In heat transfer without external source, the diffusion equation describes the temperature u in a region containing no heat sources or sinks. Whereas in mass transfer of chemicals it is used to describe the diffusion of chemicals that has a concentration $u(x, y, z, t)$ at position (x, y, z) and time t.

A one dimensional heat equation with Drichlet boundary condition is given by (Bradie, 2006)

$$\begin{aligned} \frac{\partial u}{\partial t} &= D\frac{\partial^2 u}{\partial x^2}, \quad A \leq x \leq B\,, t > 0\,, \\ u(A,t) &= u_A(t), \\ u(B,t) &= u_B(t), \\ u(x,0) &= f(x), \end{aligned} \tag{2.2.1}$$

where D is the diffusion coefficient and is assumed to be constant, $u_A(t)$ and $u_B(t)$ are concentration at points A and B, respectively. Details of numerical solutions of the diffusion equation can be found in many books and research articles. See, e.g., Fletcher (1989) and Smith (1985).

2.3 The Schrödinger equation

The time dependent Schrödinger equation is the most important partial differential equation which describes the time evolution of quantum state of a physical system.

Becerril et al. (2008) presented a finite difference methods to solve the one-dimensional time-dependent Schrödinger equation.

$$i\hbar\frac{\partial \psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + v(x,t)\psi(x,t), \tag{2.3.1}$$

where $v = 0$, except at the boundaries.

The initial and boundary conditions are given by

$$\psi(x, t = 0) = \psi_0, \tag{2.3.2}$$

$$\psi(x = 0, t) = \psi(x = 1, t) = 0; \quad x \in [0, 1]; \tag{2.3.3}$$

where m is mass of the particle, $\hbar$ is reduced Planck's constant.

2.4 The wave equation

The wave equation is also known as the equation of vibration of a string that describes propagation of waves with speed c. It usually describes waves in elasticity, aerodynamics, acoustics, and electrodynamics.

The three-dimensional wave equation is given by (Riley et al., 2006)

$$c^2\nabla^2 u = \frac{\partial^2 u}{\partial t^2}. \tag{2.4.1}$$

In the above equation, the quantity c is the speed of propagation of the waves.

Kharab and Guenther (2006) discussed a three level difference method for the following one dimensional wave equation

$$\alpha^2 \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial t^2}, \quad 0 < x < L, \quad t > 0, \tag{2.4.2}$$

subject to the boundary conditions

$$u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0, \tag{2.4.3}$$

and the initial conditions

$$u(x,0) = f(x), \quad 0 \leq x \leq L, \tag{2.4.4}$$
$$u_t(x,0) = g(x), \quad 0 \leq x \leq L. \tag{2.4.5}$$

Numerical solutions for the wave equation have been addressed by many researchers, see , e.g., Das et al. (2013), Smith (1985), Strikwerda (1989), and some of the references therein.

In this thesis we will discuss higher order finite difference methods for the above type of wave equation. As mentioned after each of the problems described above, these equations were solved numerically by different authors. However, the discussion presented in these works in higher order approximations are essential. This is therefore what we intend to discuss in the next two chapters.

3. Higher Order Finite Difference Discretization of M-D TDPDEs

The three dimensional version of the wave equation in (2.4.2) with velocity v and acoustic pressure u in homogeneous media can be written as

$$\frac{\partial^2 u}{\partial t^2} = v^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right), \quad \text{where} \quad (x, y, z, t) \in \Omega \times [0, T], \tag{3.0.1}$$

along with the initial conditions

$$u(x, y, z, 0) = f_1(x, y, z), \tag{3.0.2}$$

$$u_t(x, y, z, 0) = f_2(x, y, z), \tag{3.0.3}$$

and the boundary condition

$$u(x, y, z, t) = g(x, y, z, t). \tag{3.0.4}$$

In this chapter we will present a higher order finite difference discretization for the acoustic wave equation given in (3.0.1)-(3.0.4).

3.1 Finite difference operators

To discretize the above PDE we consider a uniform cubic grid $\Omega = [0, 1] \times [0, 1] \times [0, 1]$ equally spaced in all spacial direction with a grid spacing $h = \frac{1}{N-1}$; N is number of grid points, τ and $u_{i,j,k}$ denotes the time-step and the numerical approximation of $u(x_i, y_j, z_k, t_n)$, respectively.

The central finite difference operators for second derivatives are written as (Moin, 2010)

$$\delta_t^2 u_{i,j,k}^n \approx u_{i,j,k}^{n+1} - 2u_{i,j,k}^n + u_{i,j,k}^{n-1}, \tag{3.1.1}$$

$$\delta_x^2 u_{i,j,k}^n \approx u_{i+1,j,k}^n - 2u_{i,j,k}^n + u_{i-1,j,k}^n, \tag{3.1.2}$$

$$\delta_y^2 u_{i,j,k}^n \approx u_{i,j+1,k}^n - 2u_{i,j,k}^n + u_{i,j-1,k}^n, \tag{3.1.3}$$

$$\delta_z^2 u_{i,j,k}^n \approx u_{i,j,k+1}^n - 2u_{i,j,k}^n + u_{i,j,k-1}^n. \tag{3.1.4}$$

A higher order finite difference approximation for the second derivative is given by (Liu and Sen, 2009).

$$\frac{\partial^2 u(x_i, y_j, z_k)}{\partial x^2} \approx \frac{1}{h^2} \left[a_0 u_{i,j,k}^n + \sum_{m=1}^{M} a_m (u_{i-m,j,k}^n + u_{i+m,j,k}^n) \right] + \mathcal{O}(h^{2M}) = \frac{L_x u_{i,j,k}^n}{h^2} + \mathcal{O}(h^{2M}), \tag{3.1.5}$$

$$\frac{\partial^2 u(x_i, y_j, z_k)}{\partial y^2} \approx \frac{1}{h^2} \left[a_0 u_{i,j,k}^n + \sum_{m=1}^{M} a_m (u_{i,j-m,k}^n + u_{i,j+m,k}^n) \right] + \mathcal{O}(h^{2M}) = \frac{L_y u_{i,j,k}^n}{h^2} + \mathcal{O}(h^{2M}), \tag{3.1.6}$$

$$\frac{\partial^2 u(x_i, y_j, z_k)}{\partial z^2} \approx \frac{1}{h^2} \left[a_0 u_{i,j,k}^n + \sum_{m=1}^{M} a_m (u_{i,j,k-m}^n + u_{i+m,j,k}^n) \right] + \mathcal{O}(h^{2M}) = \frac{L_z u_{i,j,k}^n}{h^2} + \mathcal{O}(h^{2M}), \tag{3.1.7}$$

where a_0 and a_m are central difference coefficients. Some values of these coefficients are presented in Table 3.1, and the formula to find all coefficients can be found in Liu and Sen (2009).

Table 3.1: Coefficients of central difference formula

M	a_0	a_1	a_2	a_3	a_4
1	-2	1	-	-	-
2	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$	-	-
3	$-\frac{49}{18}$	$\frac{3}{2}$	$-\frac{3}{20}$	$\frac{1}{90}$	-
4	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$

Even though this approximation is accurate up to order $2M$, its not efficient because when M becomes large, the stencil that need to be computed becomes large. The standard second-order finite difference approximation for the acoustic wave equation in (3.0.1) using the above operators is

$$\frac{\delta_t^2 u_{i,j}^n}{\tau^2} = \frac{v^2}{h^2}\left(\delta_x^2 + \delta_y^2 + \delta_z^2\right) u_{i,j}^n, \tag{3.1.8}$$

$$\delta_t^2 u_{i,j}^n = r^2\left(\delta_x^2 + \delta_y^2 + \delta_z^2\right) u_{i,j}^n, \tag{3.1.9}$$

where $r = \frac{\tau v}{h}$ is the Courant–Friedrichs–Lewy(CFL) number with $h_x = h_y = h_z = h$.

3.2 Implicit finite difference method

A fourth order accurate implicit finite difference scheme for one dimensional wave equation is presented in Smith (1985). We extend the idea for two-dimensional case as discussed below.

Considering two dimensions of the wave equation given in (3.0.1), using Taylor's series expansion of $u(t+h,x,y)$ and $u(t-h,x,y)$ about the point (t,x,y) we have

$$u(t+\tau,x,y) - 2u(t,x,y) + u(t-\tau,x,y) = \tau^2\left(\frac{\partial^2 u(t,x,y)}{\partial t^2}\right) + \frac{\tau^4}{12}\left(\frac{\partial^4 u(t,x,y)}{\partial t^4}\right) + \cdots. \tag{3.2.1}$$

If u is a solution of (3.0.1), then we have the following

$$\frac{\partial^2 u}{\partial t^2} \cong v^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \tag{3.2.2}$$

and

$$\frac{\partial^4 u}{\partial t^4} \cong v^4\left(\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4}\right). \tag{3.2.3}$$

Substituting equations (3.2.2) and (3.2.3) in to equation (3.2.1) and using the notations

$$u(t+\tau,x,y) = u_{i,j}^{n+1},$$

$$u(t-\tau,x,y) = u_{i,j}^{n-1},$$

and

$$u(t,x,y) = u_{i,j}^{n},$$

we obtain

$$u_{i,j}^{n+1}-2u_{i,j}^{n}+u_{i,j}^{n-1}=v^2\tau^2\left(\frac{\partial^2 u(t,x,y)}{\partial x^2}+\frac{\partial^2 u(t,x,y)}{\partial y^2}\right)+\frac{v^4\tau^4}{12}\left(\frac{\partial^4 u(t,x,y)}{\partial x^4}+\frac{\partial^4 u(t,x,y)}{\partial y^4}\right)+\cdots \quad (3.2.4)$$

Following Strikwerda (1989) and using Taylor's series expansion we obtain

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{h^2}\left(\delta_x^2 - \frac{1}{12}\delta_x^4\right)u \quad (3.2.5)$$

and

$$\frac{\partial^2 u}{\partial y^2} = \frac{1}{h^2}\left(\delta_y^2 - \frac{1}{12}\delta_y^4\right)u. \quad (3.2.6)$$

We also have

$$\frac{\partial^4 u}{\partial x^4} = \frac{\partial^2}{\partial x^2}\left(\frac{\partial^2 u}{\partial x^2}\right) = \frac{1}{h^4}\delta_x^4 u \quad (3.2.7)$$

and

$$\frac{\partial^4 u}{\partial y^4} = \frac{\partial^2}{\partial y^2}\left(\frac{\partial^2 u}{\partial y^2}\right) = \frac{1}{h^4}\delta_y^4 u. \quad (3.2.8)$$

Substituting (3.2.5)–(3.2.8) into (3.2.4) gives a scheme which is fourth order accurate

$$u_{i,j}^{n+1} - 2u_{i,j}^{n} + u_{i,j}^{n-1} = \left(r^2\left(1+\frac{r^2-1}{12}\delta_x^2\right)\delta_x^2 + r^2\left(1+\frac{r^2-1}{12}\delta_y^2\right)\delta_y^2\right)u_{i,j}^{n}, \quad (3.2.9)$$

where $r = \frac{v\tau}{h}$ as denoted above.

Applying the operator

$$\frac{1}{(1+\frac{r^2-1}{12}\delta_x^2)(1+\frac{r^2-1}{12}\delta_y^2)},$$

to both sides of (3.2.9), we obtain

$$\left(1+\frac{r^2-1}{12}\delta_x^2\right)\left(1+\frac{r^2-1}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^{n+1} = r^2\left[\left(1-\frac{1-r^2}{12}\delta_x^2\right)\delta_y^2+\left(1-\frac{1-r^2}{12}\delta_y^2\right)\delta_x^2\right]u_{i,j}^{n}. \quad (3.2.10)$$

Equation (3.2.10) can be written as an ADI-scheme and can be referred to as **HOC-ADI**, which can be presented more precisely as,

$$\left(1-\frac{1-r^2}{12}\delta_x^2\right)u_{i,j}^{*} = r^2\left[\left(1-\frac{1-r^2}{12}\delta_x^2\right)\delta_y^2+\left(1-\frac{1-r^2}{12}\delta_y^2\right)\delta_x^2\right]u_{i,j}^{n}, \quad (3.2.11)$$

$$\left(1-\frac{1-r^2}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^{n+1} = u_{i,j}^{*}. \quad (3.2.12)$$

We have introduced the higher order finite difference alternating direction implicit scheme for two-dimensional wave equation. In the next section we will derive another higher order scheme based on Padé approximations.

3.3 A higher order finite difference scheme

In the next section we will derive another higher order scheme based on Padé(1,1) approximations.

Another higher order finite difference scheme

In this section we will drive a numerical scheme for the wave equation which is based on the padé approximation.

From Taylor's series expansion we have

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{h^2}\left(\delta_x^2 - \frac{\delta_x^4}{12} + \cdots\right) u_{i,j}^n \tag{3.3.1}$$

$$= \frac{\delta_x^2}{h^2}\left(1 - \frac{\delta_x^2}{12}\right) u_{i,j}^n + \mathcal{O}(h^4) \tag{3.3.2}$$

$$\approx \frac{1}{h^2}\frac{\delta_x^2 u_{i,j}^n}{\left(1 + \frac{\delta_x^2}{12}\right)} + \mathcal{O}(h^4). \tag{3.3.3}$$

Therefore,

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{1}{h^2}\frac{\delta_x^2 u_{i,j}^n}{\left(1 + \frac{\delta_x^2}{12}\right)} + \mathcal{O}(h^4). \tag{3.3.4}$$

Similarly the discretization in the t, y and z directions are

$$\frac{\partial^2 u}{\partial y^2} \approx \frac{1}{h^2}\frac{\delta_y^2 u_{i,j}^n}{\left(1 + \frac{\delta_y^2}{12}\right)} + \mathcal{O}(h^4), \tag{3.3.5}$$

$$\frac{\partial^2 u}{\partial t^2} \approx \frac{1}{k^2}\frac{\delta_t^2 u_{i,j}^n}{\left(1 + \frac{\delta_t^2}{12}\right)} + \mathcal{O}(k^4), \tag{3.3.6}$$

$$\frac{\partial^2 u}{\partial z^2} \approx \frac{1}{h^2}\frac{\delta_z^2 u_{i,j}^n}{\left(1 + \frac{\delta_z^2}{12}\right)} + \mathcal{O}(h^4). \tag{3.3.7}$$

substituting (3.3.4)-(3.3.6) into (3.0.1) we have

$$\frac{1}{\tau^2}\frac{\delta_t^2 u_{i,j}^n}{\left(1 + \frac{\delta_t^2}{12}\right)} = \frac{v^2}{h^2}\left(\frac{\delta_x^2 u_{i,j}^n}{\left(1 + \frac{\delta_x^2}{12}\right)} + \frac{\delta_y^2 u_{i,j}^n}{\left(1 + \frac{\delta_y^2}{12}\right)} + \frac{\delta_z^2 u_{i,j}^n}{\left(1 + \frac{\delta_z^2}{12}\right)}\right). \tag{3.3.8}$$

The scheme presented in (3.3.8) is a 4^{th}-order accurate both in time and space for the 3-dimensional acoustic wave equation based on Padé approximation.

So far we have discretized the wave equation using two approaches in the first two sections. In the next chapter we will discuss higher order finite difference schemes for two and three dimensional wave equation based on the discretization we discussed above.

4. Higher Order Compact Finite-Difference Method for M-D TDPDEs

A compact finite difference scheme comprises of adjacent point stencils of which differences are taken at the middle node, therefore typically 3, 9 and 27 nodes are used for compact finite difference descretization in one, two and three dimensions, respectively. Whereas a non-compact stencil comprises of any number of nodes which are near the vicinity of the middle node. Usually, when the order of accuracy of a non compact scheme is greater than two, then the scheme is said to be higher order. Figure 4.1 represents a compact and non-compact stencil in two-dimensions.

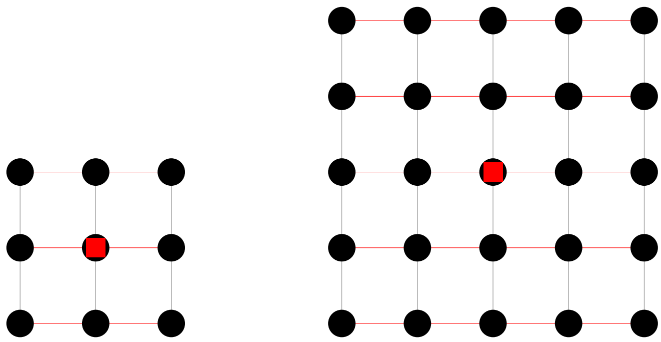

Figure 4.1: Compact (left) and Non-compact (right) stencils

4.1 Higher order compact scheme for a 2-D TDPDE

In this section we will present a higher order compact finite difference scheme for two-dimensional acoustic wave equation which was developed by Das et al. (2013).

4.1.1 Higher order compact alternating direction scheme. The standard alternating direction implicit scheme which is fourth order both in time and space is given in equation (3.2.11)-(3.2.12). Recently, Das et al. (2013) developed a low dispersive finite difference method for two-dimensional acoustic wave equation using Padé approximation, we will discuss this method in detail in this section.

Multiplying both sides of (3.3.8) by the operator

$$v^2\tau^2\left(1+\frac{1}{12}\delta_t^2\right)\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_y^2\right),$$

we get

$$(1+\frac{1}{12}\delta_x^2)(1+\frac{1}{12}\delta_y^2)\delta_t^2u_{i,j}^n = r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_y^2)\delta_x^2+(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_x^2)\delta_y^2\right]u_{i,j}^n, \quad (4.1.1)$$

which upon simplification leads to

$$\left(1+\frac{1-r^2}{12}\delta_x^2+\frac{1-r^2}{12}\delta_y^2+\frac{1-2r^2}{144}\delta_x^2\delta_y^2\right)\delta_t^2u_{i,j}^n = r^2\left(\delta_x^2+\delta_y^2+\frac{\delta_x^2\delta_y^2}{6}\right)u_{i,j}^n. \quad (4.1.2)$$

Further simplification give

$$\left(1+\frac{1-r^2}{12}\delta_x^2\right)\left(1+\frac{1-r^2}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^n - \frac{r^4}{144}\delta_x^2\delta_y^2\delta_t^2 u_{i,j}^n = r^2\left(\delta_x^2+\delta_y^2+\frac{\delta_x^2\delta_y^2}{6}\right)u_{i,j}^n. \tag{4.1.3}$$

Neglecting the term $\frac{r^4}{144}\delta_x^2\delta_y^2\delta_t^2 u_{i,j}^n$ which is equivalent to an error of $\mathcal{O}(h^6)$ we obtain the compact scheme, which is fourth order in time and space,

$$\left(1+\frac{1-r^2}{12}\delta_x^2\right)\left(1+\frac{1-r^2}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^n = r^2\left(\delta_x^2+\delta_y^2+\frac{\delta_x^2\delta_y^2}{6}\right)u_{i,j}^n. \tag{4.1.4}$$

This scheme needs to be solved in two directions simultaneously, however it is easier to solve it in one direction at a time, therefore we can write it as

$$\left(1+\frac{1-r^2}{12}\delta_x^2\right)u_{i,j}^* = r^2\left(\delta_x^2+\delta_y^2+\frac{\delta_x^2\delta_y^2}{6}\right)u_{i,j}^n, \tag{4.1.5}$$

$$\left(1+\frac{1-r^2}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^n = u_{i,j}^*. \tag{4.1.6}$$

The above scheme is based on Pad'e approximation and which can be referred to as **CPD-ADI** scheme.

Substituting (3.2.5) into (4.1.6) we obtain

$$\left(1-\frac{r^2-1}{12}\delta_y^2\right)(u_{i,j}^{n+1}-2u_{i,j}^n+u_{i,j}^{n-1}) = u_{i,j}^*. \tag{4.1.7}$$

Equation (4.1.7) is a tridiagonal system and therefore it can be solved easily by using any tri-diagonal solver.

In the next section we will derive a numerical scheme which is a combination of the compact and non-compact operators that we introduced in chapter two.

4.1.2 Hybrid scheme. The higher order compact scheme (4.1.5)–(4.1.6) derived using Padé approximation is efficient and accurate up to order 4. However the scheme suffers from a moderate numerical dispersion (Das et al., 2013). Therefore we modify the scheme by substituting one of the spacial grids (in x-direction) in equation (3.3.8) by non-compact one in equation (3.1.5) to obtain a hybrid scheme.

Therefore, for the two-dimensional wave equation we have

$$\frac{1}{\tau^2}\frac{\delta_t^2 u_{i,j}^n}{\left(1+\frac{\delta_t^2}{12}\right)} = \frac{v^2}{h^2}\left(L_x u_{i,j}^n + \frac{\delta_y^2 u_{i,j}^n}{\left(1+\frac{\delta_y^2}{12}\right)}\right). \tag{4.1.8}$$

Following the same procedure as we did for (4.1.2)–(4.1.4) we obtain

$$\left(1-\frac{r^2}{12}L_x\right)\left(1-\frac{r^2-1}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^n = \left(r^2 L_x + r^2\delta_y^2\right)u_{i,j}^n + \frac{r^2}{12}\delta_y^2 L_x u_{i,j}^n. \tag{4.1.9}$$

Therefore for implementation, this can further be written as an ADI scheme

$$\left(1-\frac{r^2}{12}L_x\right)u_{i,j}^* = r^2\left(L_x+\delta_y^2+\frac{L_x\delta_y^2}{12}\right)u_{i,j}^n, \tag{4.1.10}$$

$$\left(1-\frac{r^2-1}{12}\delta_y^2\right)\delta_t^2 u_{i,j}^n = u_{i,j}^*. \tag{4.1.11}$$

Equations (4.1.10)–(4.1.11) is an ADI scheme obtained by mixing compact and non-compact difference operators and therefore it can be referred to as non-compact padé based scheme (**NCPD-ADI**).

For the implementation, we will apply equation (4.1.10)–(4.1.11) for the interior nodes, whereas at the nodes near the horizontal boundary we will use (4.1.5)–(4.1.6). Therefore the combination of the two schemes can be called compact Padé based interlinked alternating direction implicit scheme (IPD-ADI).

4.2 Higher order compact scheme for a 3-D TDPDE

4.2.1 Higher order compact alternating direction scheme. In section 3.2, we derived higher order compact scheme for a two-dimensional wave equation. Extending (3.2.10) for three-dimensional wave equation we obtain

$$\left(1+\frac{r^2-1}{12}\delta_x^2\right)\left(1+\frac{r^2-1}{12}\delta_y^2\right)\left(1+\frac{r^2-1}{12}\delta_z^2\right)\delta_t^2 u_{i,j}^{n+1} = r^2\left[\left(1-\frac{1-r^2}{12}\delta_x^2\right)\left(1-\frac{1-r^2}{12}\delta_z^2\right)\delta_y^2 u_{i,j}^n\right] + r^2\left[\left(1-\frac{1-r^2}{12}\delta_y^2\right)\left(1-\frac{1-r^2}{12}\delta_z^2\right)\delta_x^2 u_{i,j}^n\right] + r^2\left[\left(1-\frac{1-r^2}{12}\delta_y^2\right)\left(1-\frac{1-r^2}{12}\delta_x^2\right)\delta_z^2 u_{i,j}^n\right]. \quad (4.2.1)$$

Equation (4.2.1) is 4^{th} order compact scheme, which can be implemented as

$$\left(1+\frac{r^2-1}{12}\delta_x^2\right)u_{i,j}^{**} = r^2\left[\left(1-\frac{1-r^2}{12}\delta_x^2\right)\left(1-\frac{1-r^2}{12}\delta_z^2\right)\delta_y^2 u_{i,j}^n\right] + r^2\left[\left(1-\frac{1-r^2}{12}\delta_y^2\right)\left(1-\frac{1-r^2}{12}\delta_z^2\right)\delta_x^2 u_{i,j}^n\right] + r^2\left[\left(1-\frac{1-r^2}{12}\delta_y^2\right)\left(1-\frac{1-r^2}{12}\delta_x^2\right)\delta_z^2 u_{i,j}^n\right], \quad (4.2.2)$$

$$\left(1+\frac{r^2-1}{12}\delta_y^2\right)u_{i,j}^{*} = u_{i,j}^{**}, \quad (4.2.3)$$

$$\left(1+\frac{r^2-1}{12}\delta_z^2\right)\delta_t^2 u_{i,j}^{n+1} = u_{i,j}^{*}. \quad (4.2.4)$$

Equations (4.2.2)–(4.2.4) is a HOC-ADI scheme for three-dimensional acoustic wave equation.

Now we will present a higher order compact Padé based scheme for three-dimensional wave equitation developed by Liao (2013).

Multiplying both sides of (3.3.8) by

$$v^2\tau^2\left(1+\frac{1}{12}\delta_t^2\right)\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right),$$

we obtain

$$\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\delta_t^2 u_{i,j}^n = r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_y^2)(1+\frac{1}{12}\delta_z^2)\delta_x^2\right]u_{i,j}^n + r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_x^2)(1+\frac{1}{12}\delta_z^2)\delta_y^2\right]u_{i,j}^n + r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_x^2)(1+\frac{1}{12}\delta_y^2)\delta_z^2\right]u_{i,j}^n. \quad (4.2.5)$$

Simplifying as we did earlier for (4.1.2)-(4.1.3), we obtain

$$\left(1+\frac{1-r^2}{12}\delta_x^2\right)\left(1+\frac{1-r^2}{12}\delta_y^2\right)\left(1+\frac{1-r^2}{12}\delta_z^2\right)\delta_t^2 u_{i,j}^n = r^2\left(\delta_x^2\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+r^2\left(\delta_y^2\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+r^2\left(\delta_z^2\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_y^2\right)\right)u_{i,j}^n. \quad (4.2.6)$$

Which can be written as a succession of three one dimensional problems as in the following.

$$\left(1+\frac{1-r^2}{12}\delta_x^2\right)u_{i,j}^{**} = r^2\left(\delta_x^2\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+\,r^2\left(\delta_y^2\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+\,r^2\left(\delta_z^2\left(1+\frac{1}{12}\delta_x^2\right)\left(1+\frac{1}{12}\delta_y^2\right)\right)u_{i,j}^n, \quad (4.2.7)$$

$$\left(1+\frac{1-r^2}{12}\delta_y^2\right)u_{i,j}^{*} = u_{i,j}^{**}, \quad (4.2.8)$$

$$\left(1+\frac{1-r^2}{12}\delta_z^2\right)\delta_t^2 u_{i,j}^{n+1} = u_{i,j}^{*}. \quad (4.2.9)$$

The Scheme consisting of (4.2.7)–(4.2.9) is a Padé based ADI scheme, which can be referred as **CPD-ADI** scheme for three dimensional acoustic wave equation.

In the next section we will derive a hybrid scheme developed by intermixing the compact and the non-compact operators in one of the spatial direction.

4.2.2 Hybrid scheme. In the above section we derived a scheme which is fourth order in time and space using compact operators in all directions. However to minimize dispersion we will use a non-compact operator in the x-direction.

Therefore, (3.3.8) can be written as

$$\frac{1}{\tau^2}\frac{\delta_t^2 u_{i,j}^n}{\left(1+\frac{\delta_t^2}{12}\right)} = \frac{v^2}{h^2}\left(L_x + \frac{\delta_y^2 u_{i,j}^n}{\left(1+\frac{\delta_y^2}{12}\right)} + \frac{\delta_z^2 u_{i,j}^n}{\left(1+\frac{\delta_z^2}{12}\right)}\right). \quad (4.2.10)$$

Multiplying both sides of (4.2.10) by

$$v^2\tau^2\left(1+\frac{1}{12}\delta_t^2\right)\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right),$$

we obtain

$$(1+\frac{1}{12}\delta_y^2)(1+\frac{1}{12}\delta_z^2)\delta_t^2 u_{i,j}^n = r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_y^2)(1+\frac{1}{12}\delta_z^2)\delta_x^2\right]u_{i,j}^n$$
$$+r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_z^2)\delta_y^2\right]u_{i,j}^n$$
$$+r^2\left[(1+\frac{1}{12}\delta_t^2)(1+\frac{1}{12}\delta_y^2)\delta_z^2\right]u_{i,j}^n. \quad (4.2.11)$$

Equation (4.2.11) can be written as

$$\left(1-\frac{r^2}{12}L_x\right)\left(1+\frac{1-r^2}{12}\delta_y^2\right)\left(1+\frac{1-r^2}{12}\delta_z^2\right)\delta_t^2u_{i,j}^n = r^2\left(L_x\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+r^2\left(\delta_y^2\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+r^2\left(\delta_z^2\left(1+\frac{1}{12}\delta_y^2\right)\right)u_{i,j}^n. \quad (4.2.12)$$

The factorization error we encountered in factorizing the left hand side of (4.2.11) is

$$err = \frac{r^4}{144}\left(L_x\delta_y^2 - L_x\delta_z^2 - \delta_y^2\delta_z^2 - \frac{2-r^2}{12}L_x\delta_y^2\delta_z^2\right)\delta_t^2u_{i,j}^n,$$

which is about $\mathcal{O}(h^6)$, therefore we can ignore these error terms.

Equation (4.2.12) can be written as

$$\left(1-\frac{r^2}{12}L_x\right)u_{i,j}^{**} = r^2\left(L_x\left(1+\frac{1}{12}\delta_y^2\right)\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+ r^2\left(\delta_y^2\left(1+\frac{1}{12}\delta_z^2\right)\right)u_{i,j}^n$$
$$+ r^2\left(\delta_z^2\left(1+\frac{1}{12}\delta_y^2\right)\right)u_{i,j}^n, \quad (4.2.13)$$

$$\left(1+\frac{1-r^2}{12}\delta_y^2\right)u_{i,j}^{*} = u_{i,j}^{**}, \quad (4.2.14)$$

$$\left(1+\frac{1-r^2}{12}\delta_z^2\right)\delta_t^2u_{i,j}^n = u_{i,j}^{*}. \quad (4.2.15)$$

Where (4.2.13)–(4.2.14) are three dimensional implicit alternating direction scheme obtained by intermixing the compact and the non-compact finite difference operators, therefore it can be referred as to **NCPD-ADI** scheme for the three dimensional wave equation.

At this stage, we would like to mention that a typical numerical method may produce spurious solution, a phenomena which is greatly attributed due to dispersion. Thus, in the next chapter we will study this phenomena in detail.

5. Dispersion Relation and Stability Analysis

Finite difference schemes are widely used in solving time dependent partial differential equations numerically, however in approximation of derivatives using Taylor's series, truncation of terms produces inaccuracies in finding solutions for such differential equations. Due to these inaccuracies undesirable ripples are produced in the process of discretization. Eventhough such equations are not frequency dependent, due to truncation of higher order terms frequency dependent numerical errors are produced. This numerical phenomena is called dispersion. Thus, even for non-dispersive partial differential equations their discrete approximations are dispersive. Moreover in descritizing a differential equation , depending on our interest in accuracy, we ignore higher order terms, due to these inaccuracies errors are introduced which results in instability of the finite difference scheme.

5.1 Dispersion relation

In this section we will discuss the dispersion relation in general and the numerical dispersions for the discrete solutions of wave equations for the methods that we are employing in particular.

We will consider a scalar wave equation (3.0.1) which has solution of the form

$$u(x, y, z, t) = u_0 e^{l(k_x x + k_y y + k_z z - \omega t)}, \tag{5.1.1}$$

Then its discrete form is given by

$$u^n_{i,j,m} = u_0 e^{l(k_x ih + k_y jh + k_z mh - \omega n\tau))}, \tag{5.1.2}$$

where u_0 is pressure amplitude, ω denotes angular frequency, $h_x = h_y = h_z = h$ is grid spacing, τ is time-step and discrete directional wave numbers are given by $\mathbf{k} = (k_x, k_y, k_z)$, $k_x = |\mathbf{k}|cos(\theta)\cos(\phi)$, $k_y = |\mathbf{k}|\sin(\theta)\cos(\phi)$, and $k_z = |\mathbf{k}|\sin(\phi)$ and $l = \sqrt{-1}$.

The dispersion relation is given by

$$\omega = \omega(k), \tag{5.1.3}$$

where $\omega = k.v$ is the analytical dispersion relation and we will derive the numerical dispersion relation for two and three-dimensional wave equation for the mentioned schemes.

In numerical analysis the relation between the numerical angular frequency $\bar{\omega}$ and **k**, v and numerical parameters τ and h is called numerical dispersion relation.

Dispersion error therefore can be considered as the difference between the numerical and analytical frequencies or the ratio of these frequencies. Consequently, it can be measured as the difference between, or the ratio of numerical and analytical velocities. Since the latter method is the most convenient to work with, we will use this method for our dispersion measurement. Thus, mathematically,

$$\delta = \frac{\bar{\omega}}{\omega} = \frac{\bar{v}}{v}, \tag{5.1.4}$$

where $\bar{v}$ is numerical velocity and δ is the normalized phase error.

Therefore $\delta = 1$ imply the numerical scheme that we are evaluating is non-dispersive, where as for values largely deviating from 1 indicates the scheme is dispersive.

Applying finite difference operators to (5.1.2) gives as

$$\delta_t^2 u^n i,j = -4\sin^2\left(\frac{\omega\tau}{2}\right) u^n i,j, \tag{5.1.5}$$

$$\delta_x^2 u^n i,j = -4\sin^2\left(\frac{k_x h}{2}\right) u^n i,j, \tag{5.1.6}$$

$$\delta_y^2 u^n i,j = -4\sin^2\left(\frac{k_y h}{2}\right) u^n i,j, \tag{5.1.7}$$

$$\delta_z^2 u^n i,j = -4\sin^2\left(\frac{k_z h}{2}\right) u^n i,j. \tag{5.1.8}$$

For two-dimensional HOC-ADI scheme the phase relation is derived as follows. Substituting (5.1.2) into (3.2.10) we obtain

$$-4\left(1+\frac{r^2-1}{12}s_2\right)\left(1+\frac{r^2-1}{12}s_3\right)\sin^2\left(\frac{\omega\tau}{2}\right) = r^2\left(\left(1+\frac{r^2-1}{12}s_2\right)s_3+\left(1+\frac{r^2-1}{12}s_3\right)s_2\right), \tag{5.1.9}$$

$$\sin^2\left(\frac{\omega\tau}{2}\right) = \frac{r^2\left(\left(1+\frac{r^2-1}{12}s_2\right)s_3+\left(1+\frac{r^2-1}{12}s_3\right)s_2\right)}{-4\left(1+\frac{r^2-1}{12}s_2\right)\left(1+\frac{r^2-1}{12}s_3\right)}, \tag{5.1.10}$$

$$\frac{\omega\tau}{2} = \arcsin\left[\frac{r^2\left(\left(1+\frac{r^2-1}{12}s_2\right)s_3+\left(1+\frac{r^2-1}{12}s_3\right)s_2\right)}{-4\left(1+\frac{r^2-1}{12}s_2\right)\left(1+\frac{r^2-1}{12}s_3\right)}\right]^{1/2}, \tag{5.1.11}$$

$$\delta_{HOC} = \frac{2}{rkh}\arcsin\left[\frac{r^2\left(\left(1+\frac{r^2-1}{12}s_2\right)s_3+\left(1+\frac{r^2-1}{12}s_3\right)s_2\right)}{-4\left(1+\frac{r^2-1}{12}s_2\right)\left(1+\frac{r^2-1}{12}s_3\right)}\right]^{1/2}, \tag{5.1.12}$$

Similarly the normalized phase relation for CPD and NCPD schemes in two dimensions respectively are given by

$$\delta_{CPD} = \frac{2}{rkh}\arcsin\left[\frac{r^2(s_2+s_3+\frac{s_2 s_3}{6})}{-4\left(1+\frac{1-r^2}{12}s_2\right)\left(1+\frac{1-r^2}{12}s_3\right)}\right]^{1/2}, \tag{5.1.13}$$

and

$$\delta_{NCPD} = \frac{2}{rkh}\arcsin\left[\frac{r^2\left(s_1+s_3+\frac{s_1 s_3}{12}\right)}{-4\left(1-\frac{r^2}{12}s_1\right)\left(1+\frac{1-r^2}{12}s_3\right)}\right]^{1/2}, \tag{5.1.14}$$

where

$$s_1 = a_0 + 2\sum_{m=1}^{M} a_m\cos(mk_x h/2),$$

$$s_2 = -4\sin^2(\frac{k_x h}{2}),$$

$$s_3 = -4\sin^2(\frac{k_y h}{2}),$$

$$s_4 = -4\sin^2(\frac{k_z h}{2}).$$

Similarly, for three-dimensional scheme we have

$$\delta_{HOC} = \frac{2}{rkh} \arcsin\left(S_1(s,r)\right)^{1/2}, \tag{5.1.15}$$

$$\delta_{CPD} = \frac{2}{rkh} \arcsin\left(S_2(s,r)\right)^{1/2}, \tag{5.1.16}$$

with

$$S_1(s,r) = \frac{r^2\left[\left(1-\frac{1-r^2}{12}s_2\right)\left(1-\frac{1-r^2}{12}s_4\right)s_3+\left(1-\frac{1-r^2}{12}s_3\right)\left(1-\frac{1-r^2}{12}s_4\right)s_2+\left(1-\frac{1-r^2}{12}s_3\right)\left(1-\frac{1-r^2}{12}s_2\right)s_4\right]}{-4\left(1+\frac{r^2-1}{12}s_2\right)\left(1+\frac{r^2-1}{12}s_3\right)\left(1+\frac{r^2-1}{12}s_4\right)},$$

$$S_2(s,r) = \frac{r^2\left[\left(1-\frac{1-r^2}{12}s_2\right)\left(1-\frac{1-r^2}{12}s_4\right)s_3+\left(1-\frac{1-r^2}{12}s_3\right)\left(1-\frac{1-r^2}{12}s_4\right)s_2+\left(1-\frac{1-r^2}{12}s_3\right)\left(1-\frac{1-r^2}{12}s_2\right)s_4\right]}{-4\left(1-\frac{r^2-1}{12}s_2\right)\left(1-\frac{r^2-1}{12}s_3\right)\left(1-\frac{r^2-1}{12}s_4\right)},$$

and

$$\delta_{NCPD} = \frac{2}{rkh} \arcsin\left[\frac{r^2\left[\left(1+\frac{1}{12}s_3\right)\left(1+\frac{1}{12}s_4\right)s_1+\left(1+\frac{1}{12}s_4\right)s_3+\left(1+\frac{1}{12}s_3\right)s_4\right]}{-4\left(1-\frac{r^2}{12}s_1\right)\left(1-\frac{r^2-1}{12}s_3\right)\left(1-\frac{r^2-1}{12}s_4\right)}\right]^{1/2}. \tag{5.1.17}$$

The plots for these normalized dispersion relations are given in the next chapter.

5.2 Stability analysis

A numerical scheme is said to be stable if the errors produced, due to descritization, at one time-step of the calculation do not propagate as computation continues. For a stable scheme, the errors decay and eventually damp out, whereas for the unstable scheme the errors grow with time.

In this section we will analyse stability for HOC, CPD and NCPD schemes using Von Neumann stability analysis.

Therefore, the CFL condition for the HOC scheme is derived as follows

Equation (5.1.2) can be written as

$$u^n_{i,j} = u_0 e^{-l\omega n\tau} e^{l(k_x ih + k_y jh)}, \tag{5.2.1}$$

$$= \zeta^n u_0 e^{l(k_x ih+k_y jh)}. \tag{5.2.2}$$

Substituting (5.2.2) in to (3.2.10) we obtain

$$(\zeta^{n+1} - 2\zeta^n + \zeta^{n-1})\left(1+\frac{r^2-1}{12}s_2\right)\left(1+\frac{r^2-1}{12}s_3\right) = \zeta^n r^2\left[\left(1-\frac{1-r^2}{12}s_2\right)s_3+\left(1-\frac{1-r^2}{12}s_3\right)s_2\right]. \tag{5.2.3}$$

We consider $\zeta^n = z$, then (5.2.3) can be written as

$$z^2 - \frac{2A+B}{A}z + 1 = 0, \tag{5.2.4}$$

where

$$A = \left(1 + \frac{r^2-1}{12}s_2\right)\left(1 + \frac{r^2-1}{12}s_3\right), \tag{5.2.5}$$

and

$$B = r^2\left[\left(1 - \frac{1-r^2}{12}s_2\right)s_3 + \left(1 - \frac{1-r^2}{12}s_3\right)s_2\right]. \tag{5.2.6}$$

For stability the root condition for (5.2.4) should be satisfied. Therefore,

$$-2 < \frac{2A+B}{A} < 2 \Rightarrow -4 < \frac{B}{A} < 0. \tag{5.2.7}$$

Similarly for the CPD scheme we find the stability condition as

$$-4 < \frac{B'}{A'} < 0, \tag{5.2.8}$$

where

$$A' = \left(1 - \frac{(r^2-1)}{12}s_2 - \frac{r^2-1}{12}s_3 + \frac{(r^2-1)^2}{144}s_3 s_2\right), \tag{5.2.9}$$

and

$$B' = \left(r^2 s_3 + r^2 s_2 + \frac{r^2}{6}s_1 s_2\right). \tag{5.2.10}$$

And for the NCPD scheme the stability condition is

$$-4 < \frac{B''}{A''} < 0, \tag{5.2.11}$$

where

$$A'' = \left(1 - \frac{(r^2-1)}{12}s_2 - \frac{r^2}{12}s_3 + \frac{r^2(r^2-1)}{144}s_3 s_2\right), \tag{5.2.12}$$

and

$$B'' = \left(r^2 s_3 + r^2 s_2 + \frac{r^2}{12}s_1 s_2\right). \tag{5.2.13}$$

Hence from (5.2.7), (5.2.8) and (5.2.11) we can observe that the three schemes (HOC, CPD and NCPD) are conditionally stable. Note that most of the other finite difference schemes for the acoustic wave equation are conditionally stable, see e.g., Bradie (2006), Kowalczyk and Van Walstijn (2010).

Numerical results on the dispersion relations derived above will be plotted in the next chapter.

6. Dispersion Analysis and Discussion

In chapter five, we discussed the dispersion relation for three finite difference schemes which are HOC, CPD and NCPD schemes. In the next two sections, we will provide a comparison of the dispersion relations of these schemes. We present plots of the dispersion relations as a function of propagation angle θ and number of cells per wavelength (kh) for these schemes. Therefore, we discussed the normalized phase error with respect to different parameters and we approached the comparison of the dispersion errors by plotting the norm of the errors and relative phase errors.

Normalized phase error

From the numerical dispersion relations we derived in chapter 5, we can observe that the numerical dispersion of the above mentioned methods are dependent on three variables. Therefore the normalized phase errors for these methods are studied based on these three factors.

- CFL numbers (r)
- Propagation angle (θ)
- Number of cells per wavelength (kh)

Effect of different CFL number

For the analysis given here, we keep the grid size equal in all spatial directions, i.e., $h_x = h_y = h_z = h$ and $\theta = 0$. Therefore, by varying r from 0.4 to 1.0 we plot the dispersion error for each scheme. We also used the term 'exact' in all the plots for implying that there is no dispersion error, and for NCPD scheme we considered $M = 3$ for all the plots.

Figure 6.1 shows the normalized phase error, derived in the earlier section, with respect to kh for HOC-ADI scheme. As clearly observed from the plot, the phase error decreases as CFL number increases; moreover for small kh the phase error decreases for all values of r.

In Figure 6.2 we plot the normalized phase error for CPD-ADI scheme. As we can closely observe that the plots for HOC-ADI and CPD-ADI for the given parameters shows almost same result.

In Figure 6.3, we present a plot of the normalized phase error for NCPD-ADI scheme. In this case, the plot for the phase error is different from the above two plots. For $r = 1$ the schemes doesn't show phase error for HOC and CPD schemes, whereas for NCPD scheme the plot shows significant phase error.

Effect of different propagation angles (θ)

In this subsection, we present plots of the three schemes to study the effect of propagation angle on numerical dispersion. We choose $r = 0.6$ and four different values of θ varying from $\frac{\pi}{8}$ to π.

In Figure 6.4 – Figure 6.6, we provide the normalized phase error with different propagation angles of the wave. We plotted the phase error versus kh for different values of θ varying from $\frac{\pi}{8}$ to π. As the plots shows that the propagation angle has a significant contribution for the dispersion errors. It is observed that for $\theta = \frac{\pi}{4}$ the HOC-ADI schemes have lower dispersion, whereas CPD-ADI and NCPD-ADI scheme shows low dispersion at $\theta = \frac{\pi}{2}$. It is also shown that CPD-ADI and NCPD-ADI schemes have relatively low dispersion errors for larger kh values than HOC-ADI scheme.

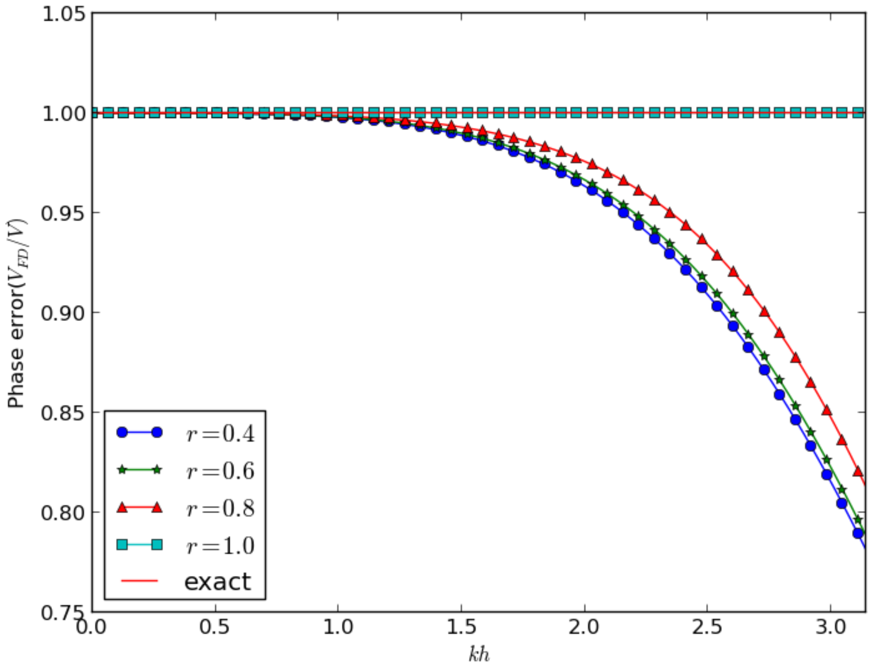

Figure 6.1: Normalized phase error for different CFL numbers for HOC-ADI scheme, $\theta = 0^o$.

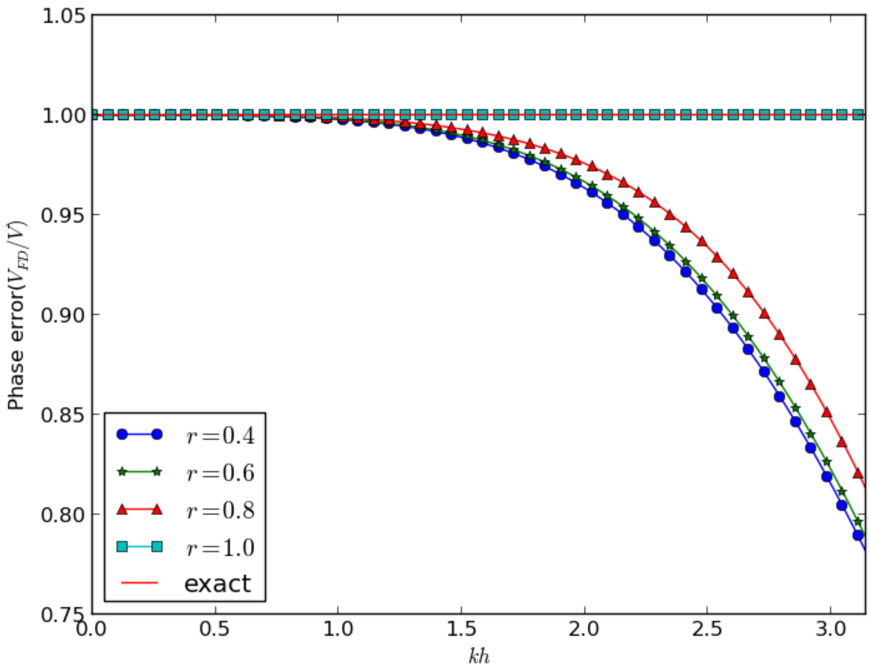

Figure 6.2: Normalized phase error for different CFL numbers for CPD-ADI scheme, $\theta = 0^o$.

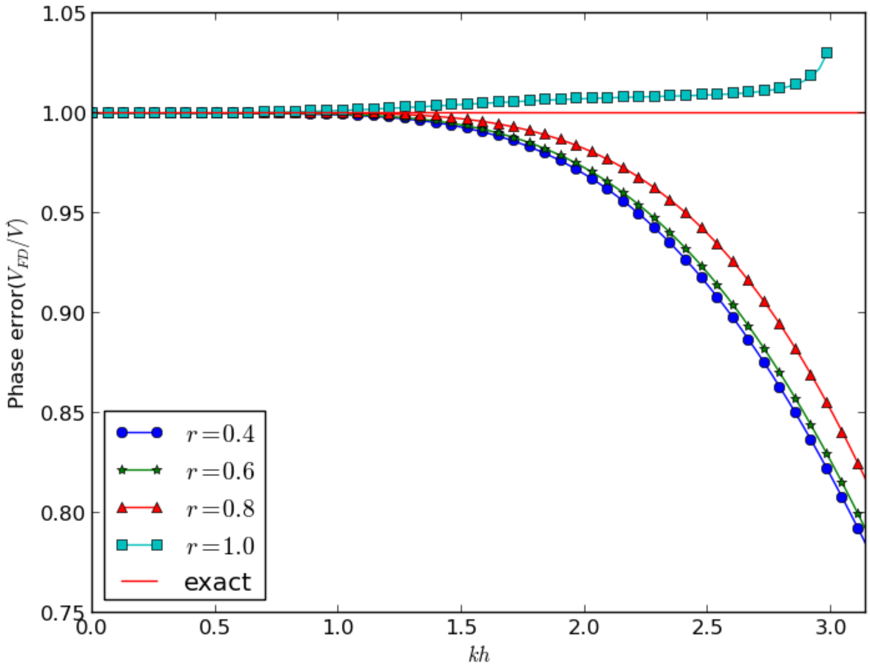

Figure 6.3: Normalized phase error for different CFL numbers for NCPD-ADI scheme, $\theta = 0^o$.

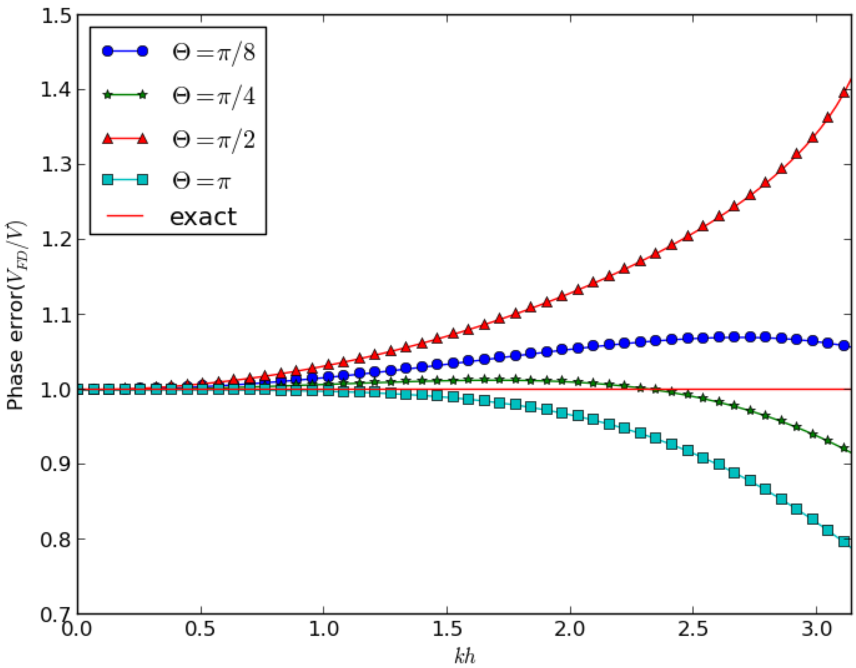

Figure 6.4: Normalized phase error for different propagation angles θ for HOC-ADI scheme, $r = 0.6$.

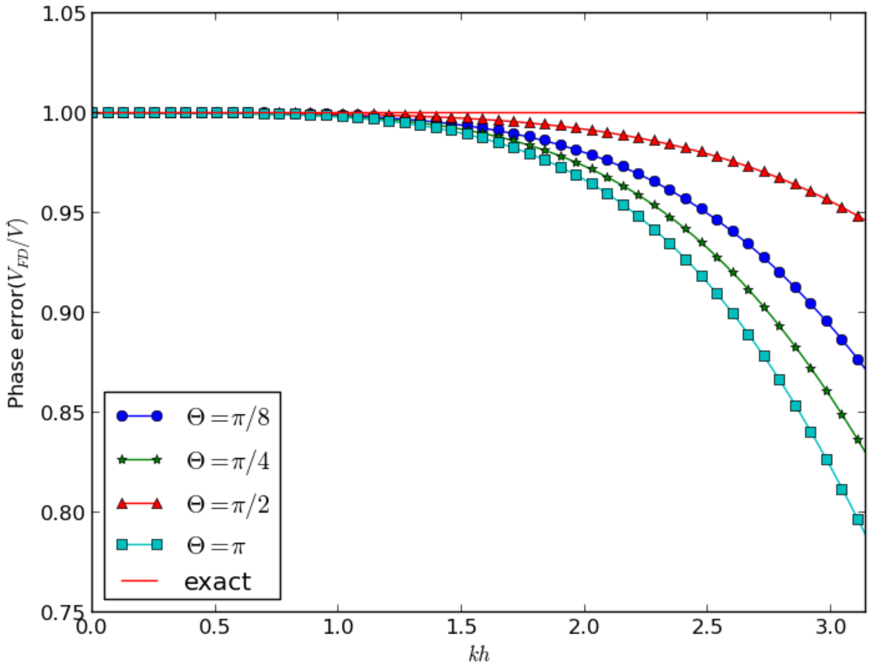

Figure 6.5: Normalized phase error for different propagation angles θ for CPD-ADI scheme, $r = 0.6$.

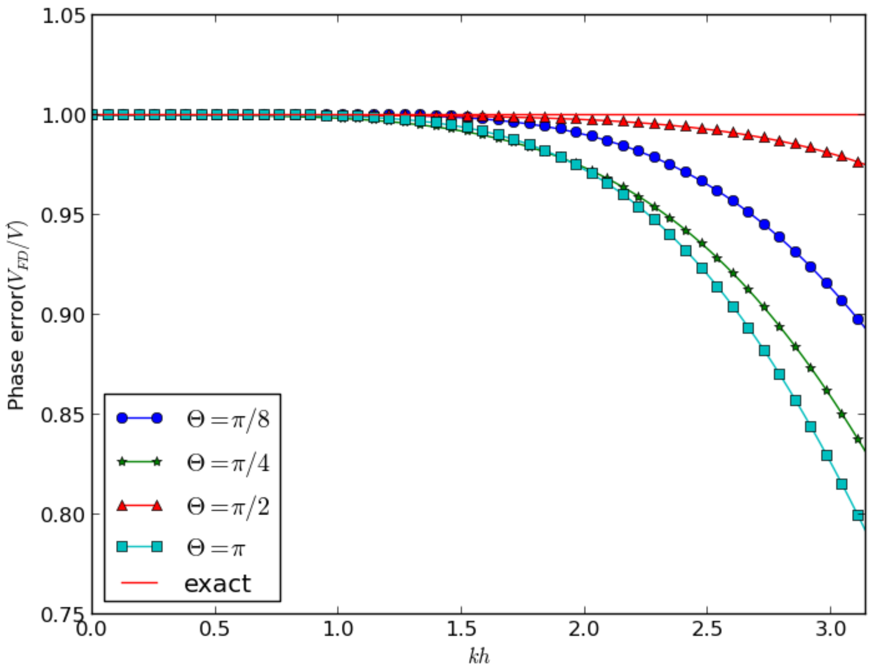

Figure 6.6: Normalized phase error for different propagation angles θ for NCPD-ADI scheme, $r = 0.6$.

Effect of different number of cells per wavelength (kh)

To examine the effect of number of cells per wavelength, we plot the dispersion errors versus θ for different values of number of cells per wavelength for the three schemes.

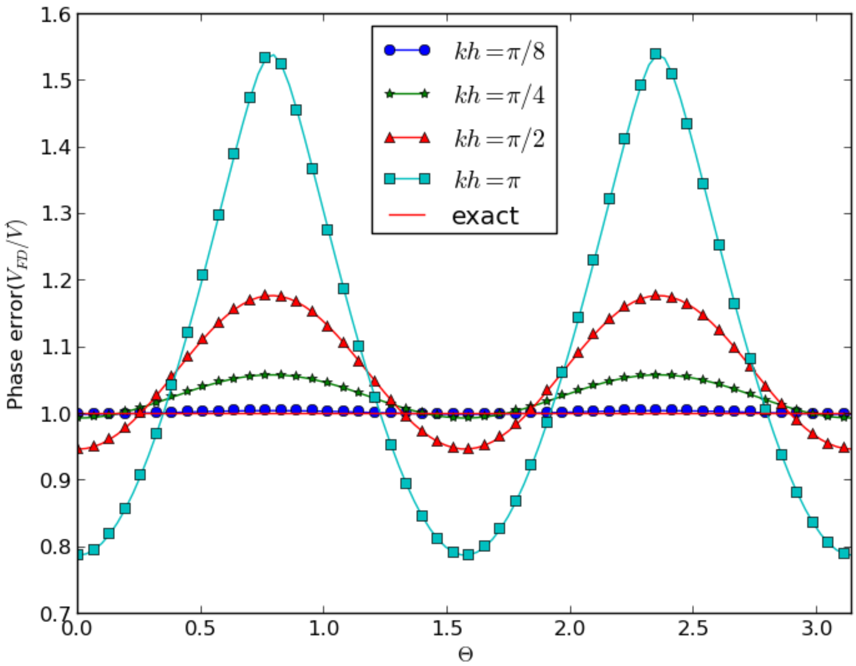

Figure 6.7: Normalized phase error for different values of kh for HOC-ADI scheme, $r = 0.6$.

In Figure 6.7–Figure 6.9 we presented the normalized phase error versus propagation angle θ for different values of kh. It is observed that the phase error increases as the propagation angle increases for all the schemes. Though all the schemes show lower dispersion error for $kh = \frac{\pi}{8}$; moreover, the CPD and NCPD schemes are relatively low dispersive for $kh = \frac{\pi}{4}$ than HOC scheme.

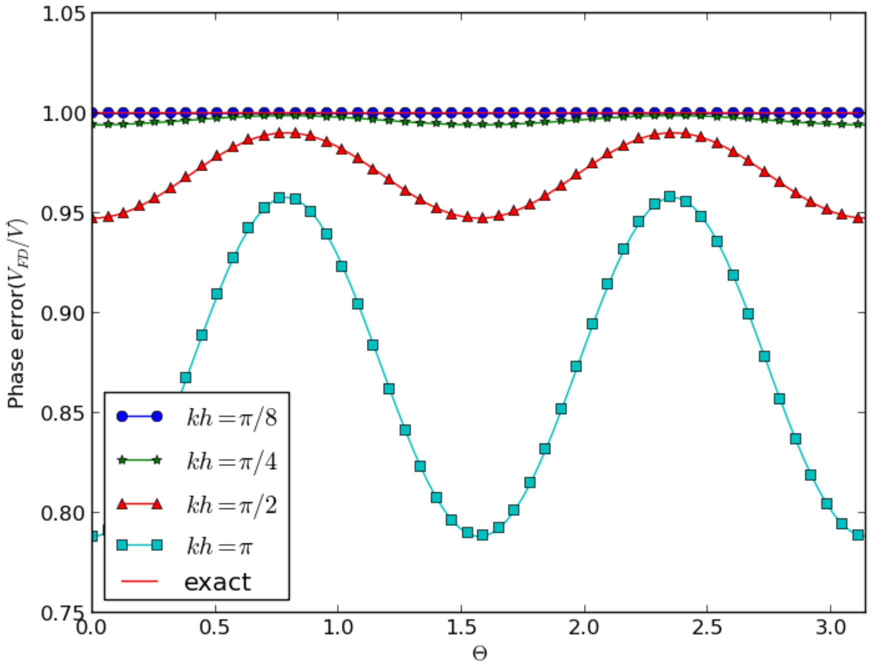

Figure 6.8: Normalized phase error for different values of kh for CPD-ADI scheme, $r = 0.6$.

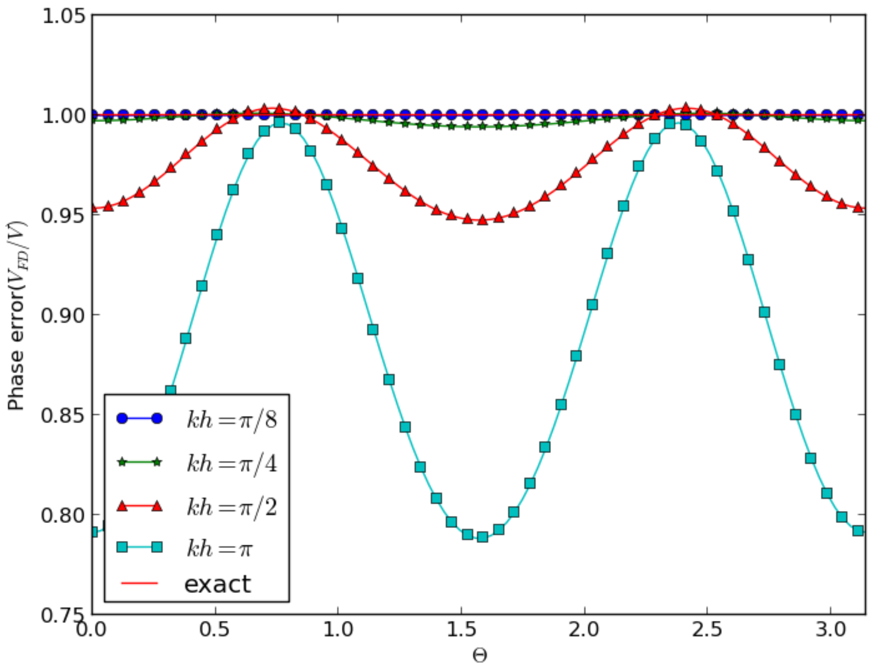

Figure 6.9: Normalized phase error for different values of kh for NCPD-ADI scheme, $r = 0.6$.

Comparison of phase error

In this section we presented plots of the L_2-norm and relative phase error for these three schemes.

Presented in Figure 6.10 is a comparison of the plots for L_2-norm for HOC-ADI, CPD-ADI and NCPD-ADI for kh ranges from 0 to π. It is clearly observed in the plot that all the schemes are periodic in θ with a period of π. It is seen in the plot that CPD and NCPD schemes have least error than HOC scheme and it is also observed that NCPD scheme has slightly smaller error than CPD scheme.

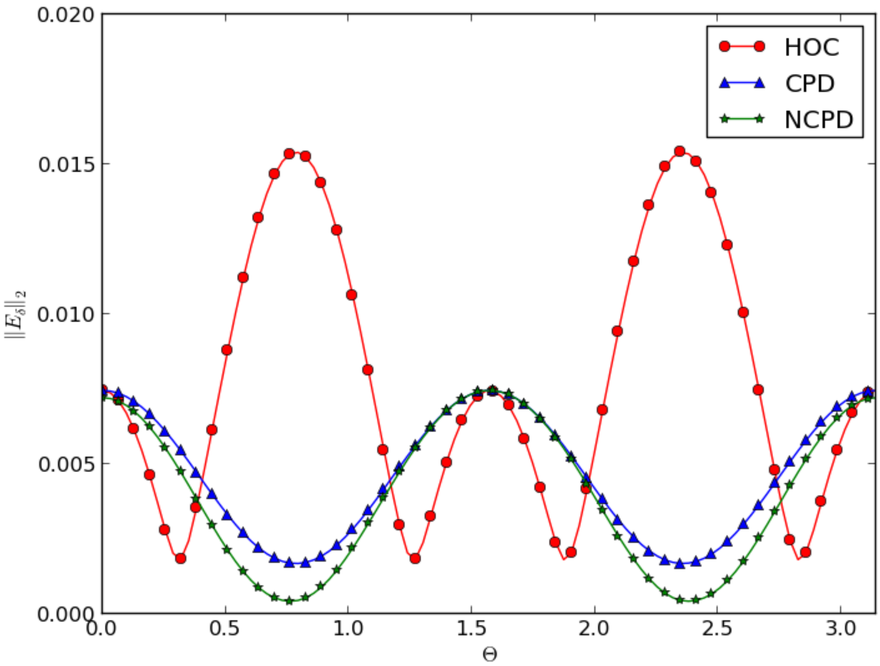

Figure 6.10: L_2-norm of normalized phase error.

The relative phase error is calculated with the following formula

$$\text{Relative error} = \frac{P_{ref} - P_{meas}}{P_{ref}}, \tag{6.0.1}$$

where P_{ref} is the reference value and P_{meas} is the numerically calculated value.

In Figure 6.11 we presented the relative phase errors of the three schemes. As can be seen on the plot, NCPD-ADI scheme has a lower dispersion errors than CPD scheme, and CPD scheme has significant lower dispersion than HOC scheme.

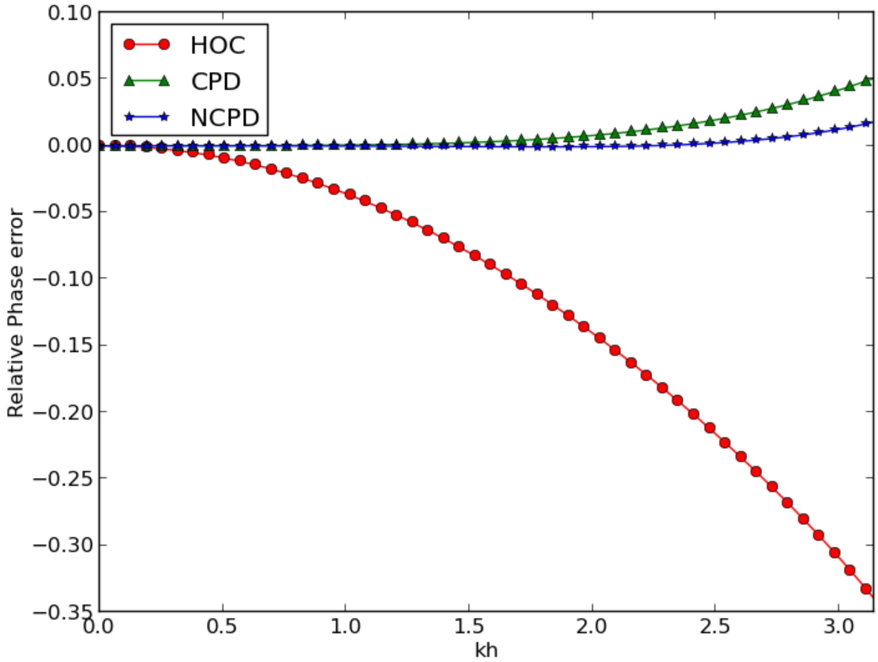

Figure 6.11: Relative phase error for HOC, CPD and NCPD schemes.

We have discussed the relative phase errors for different schemes in the individual plots above. As we have discussed in the earlier section, phase error is dependent of three factors. Therefore, it is better to see the relative phase error for the combined effect of these factors. The plots in Figure 6.12 – Figure 6.14 shows two-dimensional relative phase errors, where kh represents polar radius, θ is the polar angle and the plot shows for four values r.

From Figure 6.12 – Figure 6.14 we clearly observe that smaller r values show lower dispersion. It is also shown that waves whose propagation direction makes an angle of 45 degree with the axis are the most accurate for CPD and NCPD schemes, whereas for HOC scheme waves propagating in the axial direction shows relatively low error for some values of r. Moreover, as clearly indicated, CPD and NCPD schemes show large low dispersion region than HOC scheme.

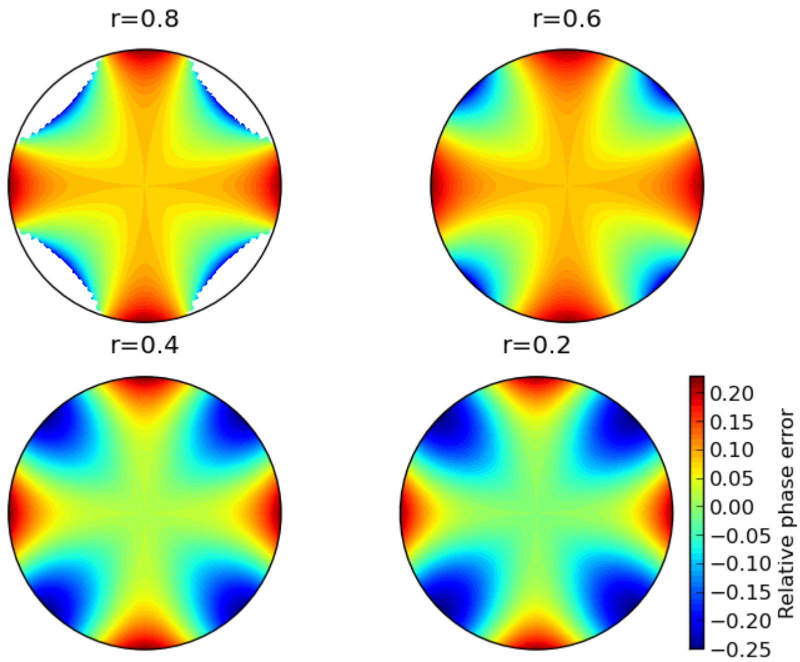

Figure 6.12: Relative phase error for HOC-ADI scheme for different values of r.

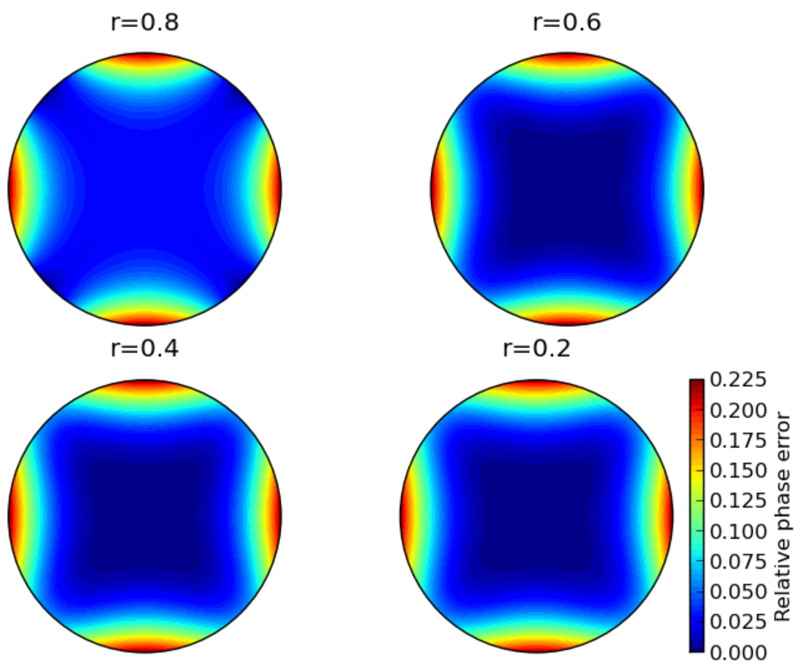

Figure 6.13: Relative phase error for CPD-ADI scheme for different values of r.

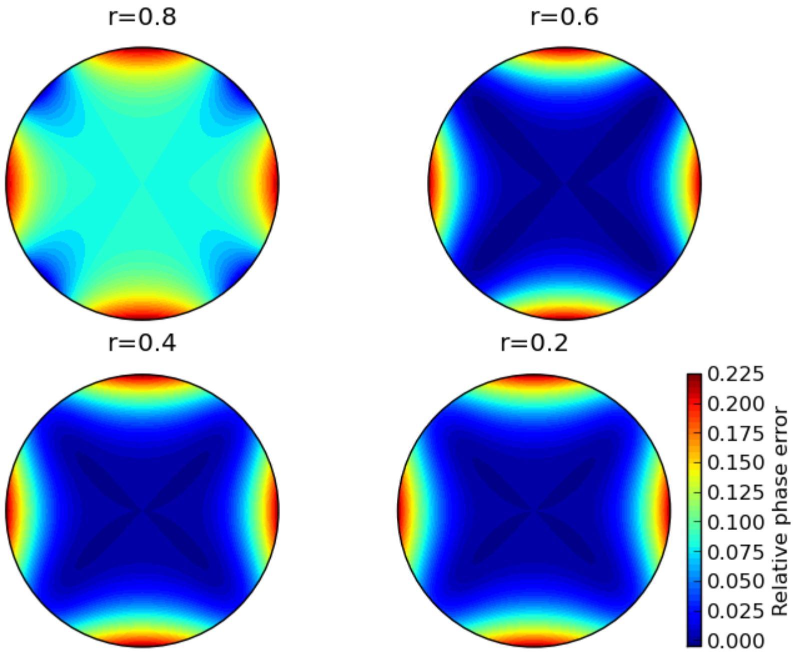

Figure 6.14: Relative phase error for NCPD-ADI scheme for different values of r.

7. Conclusion

In this thesis, three ADI schemes are presented for 2D and 3D acoustic wave equation with constant velocity. We derived HOC-ADI, CPD-ADI and NCPD-ADI schemes. The former scheme is based on Taylor approximation and the latter schemes are based on Padé approximation. We perform stability analysis for the mentioned schemes. Dispersion relations for these schemes have been also obtained followed by a thorough discussion of these relations by plotting them for different parameter sets with respect to different values of kh and θ. From this analysis, it is observed that an increase in these parameters increases the dispersion error and vice-versa. It is observed that numerical dispersion is dependent of these parameters in general for the mentioned schemes.

Comparison of phase errors for these schemes are also carried out with the given parameters. Phase error comparison of the three schemes showed that NCPD scheme has relatively lower dispersion error than CPD and HOC schemes. However, in this work we could only compare dispersion properties for three higher order numerical schemes, therefore in the future, we will analyse dispersion properties of a large group of schemes so that we will be able to explore higher order accurate low dispersive schemes.

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