Finite-Difference Methods for the Wave Equation
with Reduced Dispersion Errors

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A thesis submitted in partial fulfillment of the
requirements for the degree of

Master of Science

University of Washington

2012

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Program Authorized to Offer Degree:
Mathematics

University of Washington

Abstract

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A new methodology was proposed in Finkelstein and Kastner (2007,2008) [5,6] to derive finite-difference (FD) schemes in the joint time-space domain to reduce dispersion error. The key idea is that the true dispersion relation is satisfied exactly at some specified wavenumbers. Liu and Sen (2009) [11] further developed their idea, going to 2D and 3D. In our work, we will prove that the system for coefficients of these new schemes is solvable for any normalized wavenumbers up to the Nyquist. We will also look at the system matrix and prove that we can get higher order approximation to the dispersion at arbitrary normalized wavenumbers up to the Nyquist.

Introduction

Finite-difference-time-domain methods (FDTD) have been widely used in seismic modeling [1,14,9,7]. They are robust, simple and easy to implement, especially the second-order, centered-difference variant known as the (2,2) scheme or the Leap-frog scheme. In spite of the advantages of FD methods, the method is subject to numerical dispersion errors. Precise phase velocity can be a key factor in practice, and thus developing schemes focusing on accurate phase velocity is in demand. Traditional ways for reducing dispersion errors include increasing sampling rate and using higher-order degrees of temporal accuracy, but these methods would normally require more computation. Nonlinear methods tend to reduce dispersion errors, but they are normally not as easy to implement. To help reduce numerical dispersion with an easy-to-implement method while not increasing computation, a unified methodology has been proposed in [5] and [6] by Finkelstein and Kastner, with the key idea that schemes are obtained with the requirement that exact dispersion is prescribed at several wavenumbers of interest. Their work is based on modifications of a large class of centered Finite-Difference schemes for the wave equation. This work can accommodate arbitrary requirements for reduced phase or group velocity dispersion errors, defined over the wavenumber domain. Schemes obtained this way can give exact phase velocity at any key wavenumbers, at the cost of accuracy of the scheme, which is closely related to small dispersion error for wavenumbers near zero.

The (2,2) scheme has proved to work stably and effectively [3]. However, limits in the temporal accuracy are obvious due to its second-order approximation. Smaller time steps or smaller grid size helps to increase precision but also increases the computation. Many methods, such as high-order, staggered-grid and implicit methods have been developed to increase the accuracy while not largely complicating the computation. Here, we will focus on the technique of swapping derivatives [3], i.e., using a wider spatial stencil and thus higher spatial accuracy to compensate for the accuracy in time. Practical advantages were observed for the scalar wave equation [11,4].

In our work, we develop a unified methodology similar to the methods in [5,6,11], and we

prove that the system of coefficients obtained by the accuracy requirement at wavenumber zero accompanied with exact dispersion relations can be solved for arbitrary wavenumbers up to the Nyquist. We will also conclude that dispersion can be approximated to higher order at arbitrary wavenumbers other than zero. Our methodology is equivalent to that in [6]. However, we will prove the solvability for arbitrary wavenumbers for the first time. We will also see improvement of the dispersion approximation on the whole interval.

After a brief description of some key facts and notations, this document is devided into six sections. In the first section, we talk about the dispersion relation for wave equations and phase velocity, both for the continuous problem and for Leap-frog schemes. Section 2 introduces the traditional way of deriving a finite difference scheme and Lax-Wendroff analysis. We will see increased temporal accuracy with only three grid points in time. Section 3 presents the solvability for the coefficients for these new schemes, where exact dispersion is assigned at any wavenumber less than Nyquist. Section 4 presents numerical experiments comparing the new schemes with traditional schemes. Sections 5 and 6 sum up related work done for higher dimensions, and propose our future goals regarding group velocity angle dependence and stability analysis.

Facts and notations

1. _Vandermonde matrix_

$$
V = \begin{pmatrix}
z_1^0 & z_2^0 & \cdots & z_n^0 \\
z_1^1 & z_2^1 & \cdots & z_n^1 \\
\vdots & \vdots & \cdots & \vdots \\
z_1^{n-1} & z_2^{n-1} & \cdots & z_n^{n-1}
\end{pmatrix}
\tag{1}
$$

is called a Vandermonde matrix with determinant

$$
det(V) = \prod_{1 \leq j < k \leq n} (z_k - z_j)
$$

We will call the $\{z_l\}$'s the generating elements of the Vandermonde matrix. For simplicity, we make the convention that 1×1 Vandermonde matrix with zero generating

element has determinant 1.

2. *Chebyshev polynomials*

The Chebyshev polynomials are defined by the recurrence relation

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

They can also be defined as $T_n(x) = \cos(n \arccos x)$ for $-1 \le x \le 1$. If $x = \cos(\theta)$, then $\theta = \arccos(x)$, and $T_n(x) = \cos(n\theta)$. The Chebyshev polynomials are orthogonal in the following sense

$$\int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}} dx = \begin{cases} 0 & m \ne n, \\ \frac{\pi}{2} & m = n \ne 0, \\ \pi & m = n = 0, \end{cases}$$

so when comparing two expansions in Chebyshev polynomials, we only need to compare the coefficients for each $T_n(x)$.

3. We will use $d_M(x_1, \dots, x_j)[k_1, \dots, k_l]$ to denote the determinant of the matrix obtained from the Vandermonde matrix whose generating elements are the integers from 0^2 to M^2, with the last $j + l$ rows removed (so $p = M - (j + l)$) and replaced by j rows of Chebyshev polynomials in variables $x_1, \dots, x_j$, and with l columns removed, where

the $\{k_i\}$'s are the missing generating elements from the Vandermonde matrix.

$$d_M(x_1,\ldots,x_j)[k_1,\ldots,k_l] = \det \begin{pmatrix} 1 & 1 & \cdots & \widehat{k_1^0} & \cdots & \widehat{k_l^0} & \cdots & 1 \\ 0 & 1 & \cdots & \widehat{k_1^2} & \cdots & \widehat{k_l^2} & \cdots & M^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1^{2p} & \cdots & \widehat{k_1^{2p}} & \cdots & \widehat{k_l^{2p}} & \cdots & M^{2p} \\ 1 & T_1(x_1) & \cdots & \widehat{T_{k_1}(x_1)} & \cdots & \widehat{T_{k_l}(x_1)} & \cdots & T_M(x_1) \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 1 & T_1(x_j) & \cdots & \widehat{T_{k_1}(x_j)} & \cdots & \widehat{T_{k_l}(x_j)} & \cdots & T_M(x_j) \end{pmatrix}$$

(2)

If there is no missing element, we will just use $d_M(x_1,\ldots,x_j)$. Similarly, we use just $d_M[k_1,\ldots,k_l]$ when $j = 0$.

0.1 Dispersion relation and phase velocity

A linear dispersive equation is one that admits plane wave solutions of the form $e^{i(\omega t - \xi x)}$, with the property that the speed of propagation of these waves dependends on ξ, the wave number [12]. Specifically, the frequency ω is a function of the wave number ξ determined by the particular equation. The speed of wave propagation (or phase velocity) by definition [16] is

$$c_p(\xi) = \frac{\omega(\xi)}{\xi}$$

If the function $\omega(\xi)$ is linear, the equation is called nondispersive. To find the function $\omega(\xi)$, we take Fourier Transforms of the equation, or equivalently plug in the plane wave solution $e^{i(\omega t - \xi x)}$.

Examples

The advection equation $u_t = u_x$ has dispersion relation $\omega = \xi$.

The wave equation $u_{tt} = u_{xx}$ has dispersion relation $\omega^2 = \xi^2$, i.e. $\omega = \pm \xi$.

The heat equation $u_t = u_{xx}$ has dispersion relation $i\omega = -\xi^2$.

The Schrödginger equation $u_t = iu_{xx}$ has dispersion relation $\omega = -\xi^2$.

So the advection equation and wave equation are nondispersive, but the Schrödinger equation and the heat equation are dispersive.

Now we turn our attention to numerical methods. Even if an equation is nondispersive, a discrete model of it might be dispersive. We first look at semi-discretization of the above equations with centered differences in space and their numerical dispersion relations:

$$u_t = \frac{1}{2\Delta x}(u_{j+1} - u_{j-1}) \text{ , with } \omega = \frac{1}{\Delta x}\sin(\xi\Delta x)$$

$$u_{tt} = \frac{1}{(\Delta x)^2}(u_{j+1} + u_{j-1} - 2u_j) \text{ , with } \omega^2 = \frac{4}{(\Delta x)^2}\sin^2(\frac{\xi\Delta x}{2})$$

$$u_t = \frac{1}{(\Delta x)^2}(u_{j+1} - 2u_j + u_{j-1}) \text{ , with } i\omega = -\frac{4}{(\Delta x)^2}\sin^2(\frac{\xi\Delta x}{2})$$

$$u_t = i\frac{1}{(\Delta x)^2}(u_{j+1} - 2u_j + u_{j-1}) \text{ , with } \omega = -\frac{4}{(\Delta x)^2}\sin^2(\frac{\xi\Delta x}{2})$$

Comparison between the true and numerical dispersion relations for the examples are drawn below (Figures 1 to 4). We will always use black curves to show the true solution. We use the dot line to indicate complex solution.

As we can see, all the numerical dispersions coincides with the true dispersions near $\xi = 0$, but as wavenumbers get further away from zero, the approximations get worse.

In this work, we will develop schemes for the one dimensional wave equation

$$(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2})u = 0$$

whose purpose is to give better numerical dispersion away from zero while preserving accuracy at zero. Here $u = u(x, t)$ is the wave field and c is the true phase velocity. First take Fourier Transforms to get the dispersion relation for the continuous problem

$$\omega^2 = c^2\xi^2$$

$(t \to \omega, x \to \xi)$ Without loss of generality, we look at the rightward propagating wave with dispersion relation $\omega = c\xi$. Now ω as a function of ξ is $\omega(\xi) = c\xi$. Hence the wave equation is nondispersive with a phase velocity $c(\xi) = \frac{\omega(\xi)}{\xi} = c$. We start our analysis from the full discretization with the classical Leap-frog scheme for above equation, using 3 points
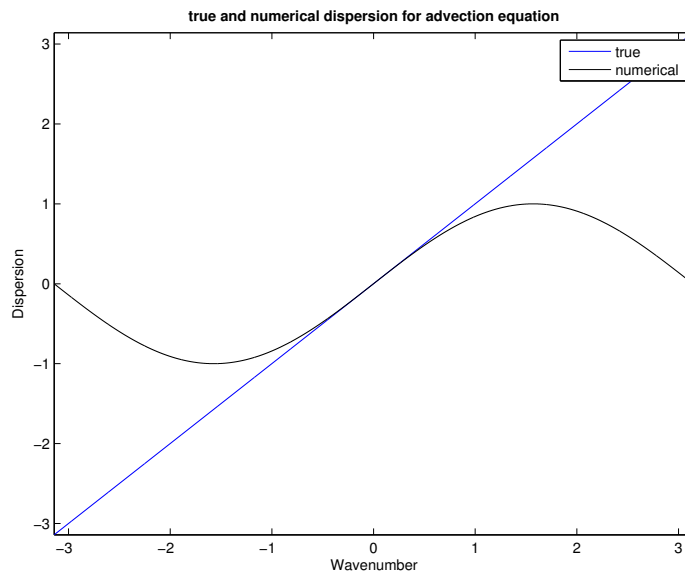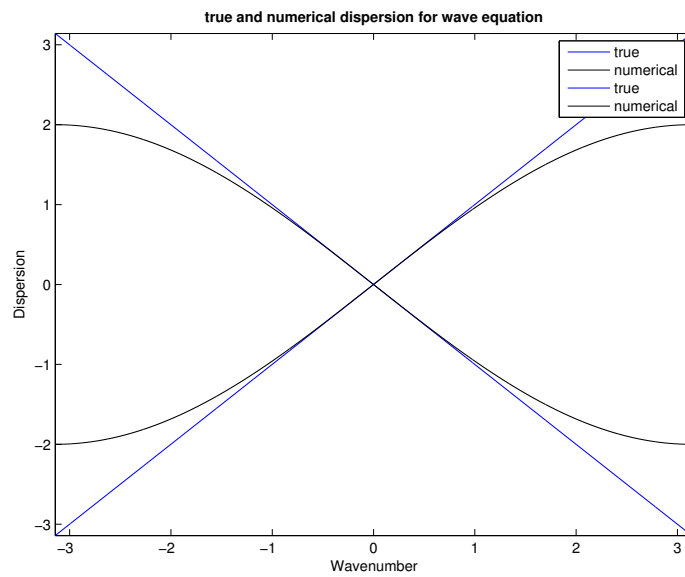
Figure 1: Advection equation
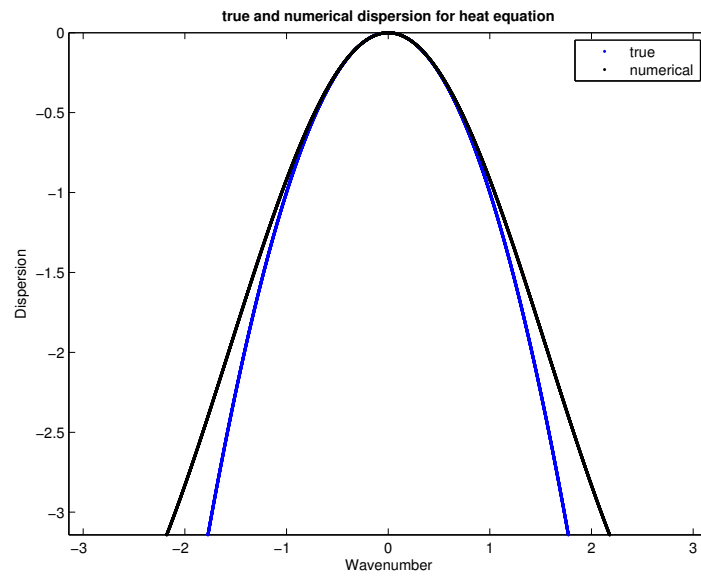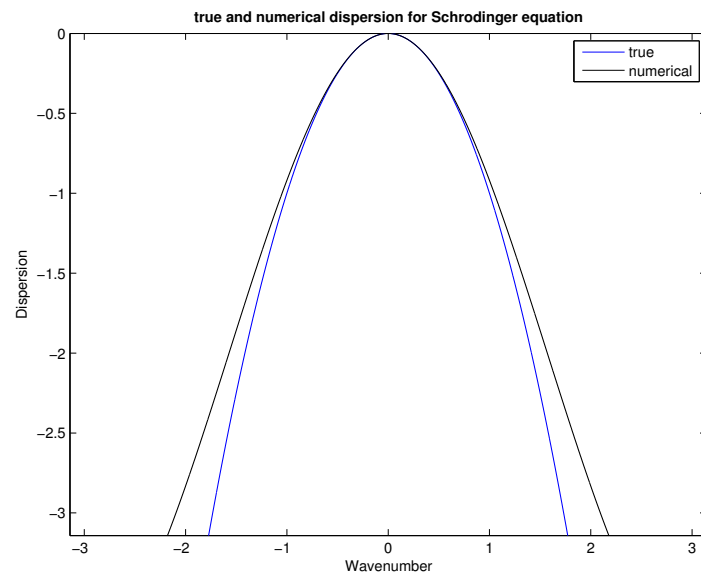

Figure 2: Wave equation

Figure 3: Heat equation

Figure 4: Schrödinger equation

respectively to approximate the 2nd order time and spatial derivatives. This leads to the following discretization

$$u_j^{n+1} - 2u_j^n + u_j^{n-1} - \gamma^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \approx 0.$$

Here $\gamma = c\frac{\Delta t}{\Delta x}$ is the CFL number, and $u_{j+m}^{n+l} = u(x + m\Delta x, t + l\Delta t)$ denotes the grid function. By taking discrete Fourier Transforms, we get the numerical dispersion relation

$$1 - \cos(\omega\Delta t) - \gamma^2 + \gamma^2\cos(\xi\Delta x) \approx 0.$$

As we can see, the numerical dispersion is multi-valued and periodic in $\xi\Delta x$ and $\omega\Delta t$. At any wavenumber $\tilde{\xi}$ above $\frac{\pi}{\Delta x}$, the wave is indistinguishable from a wave of lower wavenumber ξ, i.e., if $\tilde{\xi} = \xi + \frac{2\pi m}{\Delta x}$, we see the same wave on the grid. So it is enough to consider the values within $(\xi, \omega) \in [0, \frac{\pi}{\Delta x}] \times [0, \frac{\pi}{\Delta t}]$. The phenomenon is called aliasing, which can plague numerical computations when there are not enough spatial grid points per wavelength. The numerical phase velocity computed from above is (again we look at the rightward propagating wave)

$$c(\xi) = \frac{\omega(\xi)}{\xi} = \frac{2}{\xi\Delta t}\sin^{-1}\sqrt{\frac{c^2(\Delta t)^2}{(\Delta x)^2}\sin^2\left(\frac{\xi\Delta x}{2}\right)}$$

Just as in the semi-discrete situation, this is again a dispersive relation.

We will call $\Omega = \omega\Delta t$ the **Normalized Frequency** and $K = \xi\Delta x$ the **Normalized Wavenumber**, and $K = \pi$ is called the Nyquist wavenumber.

0.2 Accuracy analysis and finite difference

Continuing our analysis in the previous section, we will use a $(3,2M+1)$ stencil, with 3 points for temporal derivative and 2M+1 for spatial derivative. The c_m's are free coefficients in the scheme:

$$u_j^{n+1} + u_j^{n-1} + \sum_{m=0}^{M} c_m(u_{j+m}^n + u_{j-m}^n) \approx 0.$$

The benefit of a wider spatial stencil is that we can get higher temporal accuracy without having to use more time steps. This is done through Lax-Wendroff analysis, also called

derivative swapping. To illustrate this idea, let's look at accuracy of the scheme. We plug the true solution into the difference scheme to compute the local truncation error using Taylor expansions (recall $u_{j+m}^{n+l} = u(x + m\Delta x, t + l\Delta t)$):

$$LTE = u(x, t + \Delta t) + u(x, t - \Delta t) + \sum_{m=0}^{M} c_m(u(x + m\Delta x, t) + u(x - m\Delta x, t))$$

$$= \left(u(x,t) + \Delta t \frac{\partial}{\partial t} u + (\Delta t)^2 \frac{\partial^2}{\partial t^2} u + \ldots \right) + \left(u(x,t) - \Delta t \frac{\partial}{\partial t} u + (\Delta t)^2 \frac{\partial^2}{\partial t^2} u - \ldots \right)$$

$$+ 2c_0 u(x,t) + \sum_{m=1}^{M} c_m(2u(x,t) + 2(m\Delta x)^2 \frac{\partial^2}{\partial x^2} u + 2\frac{\partial^4}{\partial x^4} u + \ldots)$$

In Lax-Wendroff analysis, we replace temporal derivatives by spatial derivatives, which we can do by differentiating the original equation $(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2})u = 0$. For even orders $2k$ of derivatives, we have $(\frac{\partial^{2k}}{\partial x^{2k}} - \frac{1}{c^{2k}}\frac{\partial^{2k}}{\partial t^{2k}})u = 0$. Replacing the temporal derivatives in above equation by spatial derivatives, we get

$$LTE = 2u(x,t) + 2c^2(\Delta t)^2 \frac{\partial^2}{\partial x^2} u + \cdots + 2c_0 u(x,t)$$

$$+ \sum_{m=1}^{M} c_m(2u(x,t) + 2(m\Delta x)^2 \frac{\partial^2}{\partial x^2} u + 2\frac{\partial^4}{\partial x^4} u + \ldots)$$

$$= \left(2 + 2c_0 + \sum_{m=1}^{M} 2c_m \right) u(x,t) + \left(2(\Delta t)^2 c^2 + 2\sum_{m=1}^{M} 2c_m(m\Delta x)^2 \right) \frac{\partial^2}{\partial x^2} u$$

$$+ \left(2(\Delta t)^4 c^4 + 2\sum_{m=1}^{M} 2c_m(m\Delta x)^4 \right) \frac{\partial^4}{\partial x^4} u + \ldots$$

We make the first $p + 1$ terms vanish, dividing each equation by $(\Delta x)^{2n}$ and replacing $\frac{c\Delta t}{\Delta x}$ by γ to get:

$$2 + \sum_{m=0}^{M} 2c_m = 0,$$

$$2(\gamma^2)^j + 2\sum_{m=1}^{M} 2c_m(m^2)^j = 0, \qquad j = 1, \ldots, p.$$

Now we have accuracy of order $2p$ at (x,t) in space. But notice when $\frac{\partial^{2n}}{\partial x^{2n}}u$ vanishes, $\frac{1}{c^{2n}}\frac{\partial^{2n}}{\partial t^{2n}}u$ vanishes as well, so although we only have three grid points in the time stencil (and thus apparently only second-order accuracy in time) we are actually getting higher-order accuracy in time [4]. [6, 11] have more details on the comparison of schemes with and without Lax-Wendroff derivative swapping.

Our goal is to find a set of coefficients $\{c_m\}_{m=0}^{M}$, with required accuracy at zero and improved dispersion approximation on the whole interval up to the Nyquist wavenumber.

Applying discrete Fourier transforms in above general scheme, we get the following approximation of exact dispersion

$$\cos(\Omega) + \sum_{m=0}^{M} c_m \cos(mK) \approx 0,$$

where Ω denotes the normalized frequency and K denotes the normalized wave number as before. Let

$$\epsilon = \cos(\Omega) + \sum_{m=0}^{M} c_m \cos(mK).$$

Let's first choose to Taylor expand ϵ at $\Omega = 0$ and $K = 0$.

We get the following expansion

$$\epsilon = \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)!}(\Omega)^{2j} + \sum_{m=0}^{M} c_m \left(\sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)(mK)^{2j}} \right)$$

$$= \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)!}\left[(\Omega)^{2j} + \sum_{m=0}^{M} c_m(mK)^{2j} \right].$$

If we make the first $p+1$ terms in the infinite series vanish, we get order $2p$ accuracy of dispersion at zero. For $j = 0$, we get $1 + \sum_{m=0}^{M} c_m = 0$. For $j = 1$, $\frac{-1}{2}\left[(\Omega)^2 + \sum_{m=0}^{M} c_m(mK)^2 \right] = 0$. For general $j \geq 2$, we get $(\Omega)^{2j} + \sum_{m=0}^{M} c_m(mK)^{2j} = 0$. Plugging in the true dispersion relation $\omega^2 = c^2\xi^2$, or equivalently $\Omega = \gamma K$, and replacing the Ω in the equation above, we get $(\gamma K)^{2j} + \sum_{m=0}^{M} c_m(mK)^{2j} = 0$. This altogether gives us $p+1$ equations. From here we see that accuracy of the dispersion relation near wavenumber zero is equivalent to the usual definition of accuracy of the difference scheme at (x,t).

0.3   Dispersion reduction scheme

So far we have put $p+1$ constraints on the $\{c_m\}_{m=0}^M$, so we still need $q = (M+1) - (p+1)$ constraints to make up a $(M+1) \times (M+1)$ system. We prescribe the exact dispersion relation at q normalized wave numbers

$$\cos(K_j\gamma) + \sum_{m=0}^M c_m \cos(mK_j) = 0, \qquad j = 1, \ldots q,$$

where the domain for K_j is $(0, \pi]$.

Now we have obtained a system of $M+1$ equations in $M+1$ unknowns:

$$c_0(0^2)^0 + c_1(1^2)^0 + \ldots + c_M(M^2)^0 = -(\gamma^2)^0$$

$$c_0(0^2)^1 + c_1(1^2)^1 + \ldots + c_M(M^2)^1 = -(\gamma^2)^1$$

$$\vdots$$

$$c_0(0^2)^p + c_1(1^2)^p + \ldots + c_M(M^2)^p = -(\gamma^2)^p$$

$$c_0 + c_1 \cos(K_1) + \ldots + c_M \cos(MK_1) = -\cos(\gamma K_1)$$

$$c_0 + c_1 \cos(K_2) + \ldots + c_M \cos(MK_2) = -\cos(\gamma K_2)$$

$$\vdots$$

$$c_0 + c_1 \cos(K_q) + \ldots + c_M \cos(MK_q) = -\cos(\gamma K_q).$$

Equivalently,

$$
\begin{pmatrix}
1 & 1 & \cdots & 1 \\
0 & 1 & \cdots & M^2 \\
\vdots & \vdots & \cdots & \vdots \\
0 & 1^{2p} & \cdots & M^{2p} \\
1 & \cos(K_1) & \cdots & \cos(MK_1) \\
\vdots & \vdots & \cdots & \vdots \\
1 & \cos(K_q) & \cdots & \cos(MK_q)
\end{pmatrix}
\begin{pmatrix}
c_0 \\
c_1 \\
\vdots \\
c_p \\
c_{p+1} \\
\vdots \\
c_M
\end{pmatrix}
=
\begin{pmatrix}
-(\gamma^2)^0 \\
-(\gamma^2)^1 \\
\vdots \\
-(\gamma^2)^p \\
-\cos(\gamma K_1) \\
\vdots \\
-\cos(\gamma K_q)
\end{pmatrix}. \tag{3}
$$

To obtain a new scheme with exact dispersion at $\{K_j\}$, we solve the system above for $\{c_j\}$.

Conjecture The system above has a unique solution for all distinct $\{K_j\}_1^q$ in $(0, \pi]$. Furthermore, the determinant of the coefficient matrix is

$$\alpha_M \prod_{j=1}^{q} (1 - \cos(K_j))^{p+1} \prod_{1 \leq m < k \leq q} (\cos(K_k) - \cos(K_m)),$$

where α_M is a constant only depending on the order of matrix.

If $q = 0$ in above system, we only put restrictions on accuracy at $K = 0$, and the coefficient matrix is a Vandermonde matrix, which is invertible since the generating elements are $0^2, 1^2, \ldots, M^2$, which are all distinct. [11]

0.3.1 Specify exact phase velocity at one wavenumber

To begin with, let's consider the case where only one exact dispersion relation is required. Our coefficient matrix looks like

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & M^2 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 1^{2(M-1)} & \cdots & M^{2(M-1)} \\ 1 & \cos(K) & \cdots & \cos(MK) \end{pmatrix} \tag{4}$$

Proposition The matrix above is invertible for all K in $(0, \pi]$, and its determinant is equal to

$$d_M(x) = \alpha_M (1 - \cos(K))^M,$$

where the constant $\alpha_M = (-1)^M 2^{M-1} d_{M-1}$ only depends on the dimension M.

Letting x denote $\cos(K)$ and using the notation of Chebyshev polynomials, to compute $d_M(x)$, we can expand the matrix in to the last row (see below), and can thus write the determinant as a linear combination of Chebyshev polynomials.

To get the constant α_M, we just need to compare the leading coefficient in $d_M(x)$ and $(1 - x)^M$. For the determinant, since T_j has leading coefficient 2^{j-1}, and the highest order

of T_j is M when expanding according to the last entry of the last row. Thus we know that $(-1)^{2M}d_{M-1}T_M(x)$ and $\alpha_M(1-x)^M$ have the same leading coefficient and we conclude that $\alpha_M = (-1)^M d_{M-1}2^{M-1}$.

Proof. We prove the relation by proving that the two sides of the equation have the same induction relations, with the same initial value. For $M = 1$,

$$d_1(x) = \begin{pmatrix} 1 & 1 \\ 1 & \cos(K) \end{pmatrix} = \cos(K) - 1 \tag{5}$$

$$\alpha_1(1 - \cos(K))^1 = (-1)^1 2^{1-1}d_0(x)(1 - \cos(K))^1 = \cos(K) - 1$$

The induction relation on the polynomial side is simple:

$$\alpha_M(1 - x)^M = \alpha_M(1 - x)^{M-1}(1 - x) = \alpha_{M-1}(1 - x)^{M-1}(1 - x)\frac{\alpha_M}{\alpha_{M-1}}.$$

So to prove the result, we only need to show $d_M(x) = \frac{\alpha_M}{\alpha_{M-1}}(1 - x)d_{M-1}(x)$

We compute the determinant of the matrix of order $(M + 1) \times (M + 1)$, expand by the last row to get

$$d_M(x) = \sum_{j=0}^{M}(-1)^{M+1+j+1}\cos(jK)d_M[j] = \sum_{j=0}^{M}(-1)^{M+1+j+1}T_j(x)d_M[j]$$

We compute $(1 - x)d_{M-1}(K)$ to get

$$(1 - x)d_{M-1}(x)$$

$$= (1 - x)\sum_{j=0}^{M-1}(-1)^{M+j+1}\cos(jK)d_{M-1}(x)[j]$$

$$= \sum_{j=0}^{M-1}(-1)^{M+j+1}(1 - x)T_j(x)d_{M-1}(x)[j]$$

Here we use the recursion relation listed above for Chebyshev polynomials, reorganize to

get

$$(1 - x)d_{M-1}(x) = \left[(-1)^{M-1}d_{M-1}[0] - \frac{1}{2}(-1)^{M-1+0+1}d_{M-1}[1]\right]T_0(x)+$$

$$\left[(-1)^M d_{M-1}[1] - (-1)^{M-1}d_{M-1}[0] - \frac{1}{2}(-1)^{M-1}d_{M-1}[2]\right]T_1(x)+$$

$$\sum_{k=2}^{M-2}\left[(-1)^{M-1+k}d_{M-1}[k] - \frac{1}{2}(-1)^{M-1+k+1}d_{M-1}[k+1] - \frac{1}{2}(-1)^{M-1+k-1}d_{M-1}[k-1]\right]T_k(x)$$

$$+\left[(-1)^{M-1+M}d_{M-1}[M-1] - \frac{1}{2}(-1)^{M-1+M-1}d_{M-1}[M-2]\right]T_{M-1}(x)-$$

$$\frac{1}{2}(-1)^{M-1+M}d_{M-1}[M-1]T_M(x)$$

To show $d_M(x) = \frac{\alpha_M}{\alpha_{M-1}}(1-x)d_{M-1}(x)$, notice that Chebyshev polynomials are orthogonal, so we compare the coefficients term by term.

By direct computation, we see that result holds for $k = 0, 1, M-1$ and M,i.e.

$$(-1)^{M+1+0+1}T_0(x)d_M[0] = \left((-1)^{M-1}d_{M-1}[0] - \frac{1}{2}(-1)^{M-1+1}d_{M-1}[1]\right)T_0(x)$$

etc. Now for the general case, first notice that d_{M-1} and all the $\{d_{M-1}[k]\}$'s are Vandermonde matrices. We use the fact that

$$d_{M-1} = d_{M-2}\prod_{0 \le l \le M-2}((M-1)^2 - l^2) = d_{M-1}[M-1]\prod_{0 \le l \le M-2}((M-1)^2 - l^2) \qquad (6)$$

and

$$d_{M-1} = d_{M-1}[k]\prod_{0 \le l \le k-1}(k^2 - l^2)\prod_{k+1 \le l \le M-1}(l^2 - k^2) \qquad (7)$$

To simplify, we compute the right hand side of above equation

$$\prod_{0 \le l \le k-1}(k^2 - l^2)\prod_{k+1 \le l \le M-1}(l^2 - k^2)$$

$$= \prod_{0 \le l \le k-1}(k-l)\prod_{0 \le l \le k-1}(k+l)\prod_{k+1 \le l \le M-1}(l-k)\prod_{k+1 \le l \le M-1}(l+k)$$

$$= \left(\prod_{1 \le l \le k}l\right)\left(\prod_{k \le l \le 2k-1}l\right)\left(\prod_{1 \le l \le M-1-k}l\right)\left(\prod_{2k+1 \le l \le M-1+k}l\right)$$

$$= \frac{1}{2}(M-1-k)!(M-1+k)! \qquad (8)$$

Similarly

$$\prod_{0 \le l \le M-2} ((M-1)^2 - l^2) = \left(\prod_{1 \le l \le M-1} l \right) \left(\prod_{M-1 \le l \le 2M-3} l \right) = \frac{1}{2}(2(M-1))! \qquad (9)$$

Now plug (7) and (8) back into (5) and (6), equate (5) and (6) to obtain

$$\frac{d_{M-1}[k]}{d_{M-2}} = \binom{2(M-1)}{(M-1)-k}$$

We look at $d_M[k]$ in the similar way and obtain $d_M[k] = d_{M-1} \binom{2M}{M-k}$

Finally, we compute the k-th term of $d_M[x] / \left(\frac{\alpha_M}{\alpha_{M-1}} (1-x) d_{M-1} \right)$

$$d_M[k] / \left(\frac{2d_{M-1}}{d_{M-2}} \left[d_{M-1}[k] + \frac{1}{2} d_{M-1}[k+1] + \frac{1}{2} d_{M-1}[k-1] \right] \right)$$

$$= d_M[k] / \left(2d_{M-1} \left[\binom{2(M-1)}{M-1-k} + \frac{1}{2} \binom{2(M-1)}{M-1-(k+1)} + \frac{1}{2} \binom{2(M-1)}{M-1-(k-1)} \right] \right)$$

$$= d_{M-1} \binom{2M}{M-k} / \left(2d_{M-1} \left[\binom{2(M-1)}{M-1-k} + \frac{1}{2} \binom{2(M-1)}{M-1-(k+1)} + \frac{1}{2} \binom{2(M-1)}{M-1-(k-1)} \right] \right)$$

$$= 1$$

$$(10)$$

So far, we have proven that two sides satisfy the same induction relation, with the same initial value, as desired. □

0.3.2 Specify exact phase velocity at two distinct wavenumbers

Now we go up to two exact dispersion restrictions. The following matrix will be of concern:

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & M^2 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\ 1 & \cos(K_1) & \cdots & \cos(MK_1) \\ 1 & \cos(K_2) & \cdots & \cos(MK_2) \end{pmatrix} \qquad (11)$$

Our claim is that this matrix is invertible for all distinct K_j's from $(0, \pi)$, with determinant $\alpha_M (1 - \cos(K_1))^{M-1} (1 - \cos(K_2))^{M-1} (\cos(K_2) - \cos(K_1))$. Moreover, by comparing the highest order term, we get the constant $\alpha_M = 2^{2M-3} d_{M-2}$

For this case, we will again use Chebyshev polynomials, let $\cos(K_1) = T(x)$ and $\cos(K_2) = T(y)$. We will directly expand both sides in Chebyshev polynomials, compare the coefficients of corresponding terms and show that they are equal. Now since we have two angles, we will need Chebyshev polynomials in two variables. By $Stone - Weiestrass$ Theorm, we see that $\{T_k(x)T_j(y)\}$ form a orthogonal basis for the polynomial space of two variables. We will need to use the result for the previous case.

Proof. We compute the (k, j)-th coefficient in the determinant under Chebyshev polynomial expansion for $d_M(x, y)$

We expand $d_M(x, y)$ in the last row first to get

$$d_M(x, y) = \sum_{j=0}^{M} (-1)^{M+1+j+1} T_j(y) d_M(x)[j]$$

For a fixed j, we expand $d_M(x)[j]$ by the last row.

$$d_M(x)[j] = \det \begin{pmatrix} (0^2)^0 & \cdots & \widehat{(j^2)^0} & \cdots & ((M)^2)^0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (0^2)^{M-2} & \cdots & \widehat{(j^2)^{M-2}} & \cdots & ((M)^2)^{M-2} \\ T_0(x) & \cdots & \widehat{T_j(x)} & \cdots & T_M(x) \end{pmatrix} = \quad (12)$$

$$\sum_{k=0, k \neq j}^{M} (-1)^{M+k+1} T_k(x) \det \begin{pmatrix} (0^2)^0 & \cdots & \widehat{(k^2)^0} & \cdots & \widehat{(j^2)^0} & \cdots & ((M)^2)^0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ (0^2)^{M-2} & \cdots & \widehat{(k^2)^{M-2}} & \cdots & \widehat{(j^2)^{M-2}} & \cdots & ((M)^2)^{M-2} \end{pmatrix}$$

$$(13)$$

Hence the (k, j)-th term in Chebyshev polynomial with $k \neq j$ has coefficient $(-1)^{k+j+1} d_M[k, j]$

Notice

$$d_M = d_M[j] \prod_{j+1 \leq l \leq M} (l^2 - j^2) \prod_{0 \leq l \leq j-1} (j^2 - l^2)$$

and

$$d_M[j] = d_M[k, j] \prod_{0 \leq l \leq k-1} (k^2 - l^2) \prod_{k+1 \leq l \leq M, l \neq j} (l^2 - k^2)$$

Together we obtain

$$d_M = d_M[k,j] \prod_{j+1 \leq l \leq M} (l^2 - j^2) \prod_{0 \leq l \leq j-1} (j^2 - l^2) \prod_{0 \leq l \leq k-1} (k^2 - l^2) \prod_{k+1 \leq l \leq M, l \neq j} (l^2 - k^2)$$

Now we expand the terms and simplify to get

$$d_M[k,j] = \frac{4(j^2 - k^2)d_M}{(M+j)!(M-j)!(M+k)!(M-k)!}$$

Now we compute the (k,j)-th term on the polynomial side. Notice we already have the Chebyshev expansion for $(1-x)^M$ in case $q = 1$.

$$\alpha_M(1-x)^{M-1}(1-y)^{M-1}(y-x)$$

$$= 2^{2M-3}d_{M-2}\left(\frac{1}{(-1)^M 2^{M-2}d_{M-2}} \sum_{j=0}^{M-1} (-1)^{M+j+1}T_j(x)d_{M-1}[j] \times \right.$$

$$\sum_{k=0}^{M-1}(-1)^{M+k+1}T_k(y)d_{M-1}[k](y-x))$$

$$= \frac{(-1)^{j+k+1}}{d_{M-2}}(d_{M-1}[j](d_{M-1}[k+1]+d_{M-1}[k-1])-d_{M-1}[k](d_{M-1}[j+1]+d_{M-1}[j-1]))$$

$$= (-1)^{k+j+1}d_{M-2}\left(\binom{2(M-1)}{M-j}\binom{2(M-1)}{M-(k+1)} + \binom{2(M-1)}{M-j}\binom{2(M-1)}{M-(k-1)} - \right.$$

$$\left.\binom{2(M-1)}{M-k}\binom{2(M-1)}{M-(j+1)} - \binom{2(M-1)}{M-k}\binom{2(M-1)}{M-(j-1)}\right))$$

(14)

To prove the equality, we compute the ratio of the (k,j)-th term in $d_M(x,y)$ and $\alpha_M(1-x)^{M-1}(1-y)^{M-1}(y-x)$

$$ratio = \frac{4d_M}{d_{M-2}((2M)!)^2 2M(2M-1)} = 1$$

□

Remark For the $q = 2$ case, we have more boundary terms to check. Including the case where $|k - j| = 1$, and at least one of k and j is 0,1, $M - 1$ or M. But all of these cases are easy to justify.

0.3.3 Higher order approximation of dispersion relation at wavenumber away from zero

We begin our analysis from the following equation

$$
\det \begin{pmatrix}
1 & 1 & \cdots & 1 \\
0 & 1 & \cdots & M^2 \\
\vdots & \vdots & \cdots & \vdots \\
0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\
1 & \cos(K_1) & \cdots & \cos(MK_1) \\
0 & \frac{\cos(K_2)-\cos(K_1)}{K_2-K_1} & \cdots & \frac{\cos(MK_2)-\cos(MK_1)}{K_2-K_1}
\end{pmatrix}
\tag{15}
$$

$$
= \frac{1}{K_2 - K_1} \det \begin{pmatrix}
1 & 1 & \cdots & 1 \\
0 & 1 & \cdots & M^2 \\
\vdots & \vdots & \cdots & \vdots \\
0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\
1 & \cos(K_1) & \cdots & \cos(MK_1) \\
0 & \cos(K_2) - \cos(K_1) & \cdots & \cos(MK_2) - \cos(MK_1)
\end{pmatrix}
\tag{16}
$$

$$
= \frac{1}{K_2 - K_1} \det \begin{pmatrix}
1 & 1 & \cdots & 1 \\
0 & 1 & \cdots & M^2 \\
\vdots & \vdots & \cdots & \vdots \\
0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\
1 & \cos(K_1) & \cdots & \cos(MK_1) \\
1 & \cos(K_2) & \cdots & \cos(MK_2)
\end{pmatrix}
\tag{17}
$$

Take any $K_1 \neq 0, \pi$, and let $K_2 \to K_1$, use the explicit formula we have for the determinants, we get the following limit

$$\lim_{K_2 \to K_1} \det \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & M^2 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\ 1 & \cos(K_1) & \cdots & \cos(MK_1) \\ 0 & \frac{\cos(K_2)-\cos(K_1)}{K_2-K_1} & \cdots & \frac{\cos(MK_2)-\cos(MK_1)}{K_2-K_1} \end{pmatrix}$$

$$= \lim_{K_2 \to K_1} \frac{1}{K_2 - K_1} \det \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & M^2 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\ 1 & \cos(K_1) & \cdots & \cos(MK_1) \\ 1 & \cos(K_2) & \cdots & \cos(MK_2) \end{pmatrix}$$

$$= \lim_{K_2 \to K_1} \frac{1}{K_2 - K_1} \alpha_M (1 - \cos(K_1))^{M-1}(1 - \cos(K_2))^{M-1}(\cos(K_2) - \cos(K_1))$$

$$= -\alpha_M \sin(K_1)(1 - \cos(K_1))^{2M-2}$$

This expression is non-zero. On the other hand, the limit above is also

$$\lim_{K_2 \to K_1} \det \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & M^2 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\ 1 & \cos(K_1) & \cdots & \cos(MK_1) \\ 0 & \frac{\cos(K_2)-\cos(K_1)}{K_2-K_1} & \cdots & \frac{\cos(MK_2)-\cos(MK_1)}{K_2-K_1} \end{pmatrix}$$

$$= \det \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & M^2 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 1^{2(M-2)} & \cdots & M^{2(M-2)} \\ 1 & \cos(K_1) & \cdots & \cos(MK_1) \\ 0 & \sin(K_1) & \cdots & M\sin(MK_1) \end{pmatrix}$$

Now we have a new coefficient matrix, which is again invertible. Computing coefficients from here would give us order 1 approximation of the dispersion curve. Numerical demonstration is shown below.

0.4 Numerical experiments and stability criteria

We first look at stability criteria. Our scheme should look like

$$u_j^{n+1} + u_j^{n-1} + \sum_{m=0}^{M} c_m \left(u_{j-m}^n + u_{j+m}^n \right) = 0$$

Do von Neumann analysis, plug in $u_j^n = (e^{iK})^j g^n$ to get

$$g^2 + 2 \left(\sum_{m=0}^{M} c_m \cos(mK) \right) g + 1 = 0$$

For $|g| \leq 1$, we let $|\sum_{m=0}^{M} c_m \cos(mK)| \leq 1$, all $K \in [0, \pi]$.

In this section, we will do experiments for traditional scheme where all c_j's were determined by accuracy at $(K, \Omega) = (0, 0)$; then for the new scheme, we put the constraints at $K = \frac{\pi}{2}$, for both only one exact disperson and two exact dispersions. Finally we demonstrate the higher order approximation of phase velocity curve with result from Section 3.3. For all the wave propagation experiments, we will use $u(x, 0) = \sin(2\pi\xi x)$ as our initial wave signal, even number of interior points, and periodic boundary conditions. We will use the sampling rate of 4 grid points per wavelength, and $\gamma = 0.6$. We let the wave propagate on the interval of $[0, 3]$, but for the purpose of demonstration, only draw the blow-up on $[0, 0.2]$. The true wave is drawn in black for comparison. Max error `e_traditional` is the
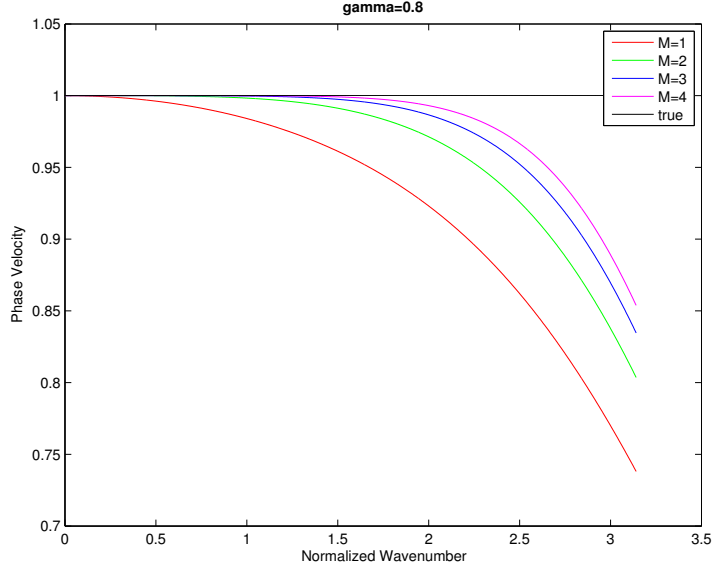
Figure 5: Velocity curves, $\gamma = 0.8$ Traditional scheme

L^∞ distance between the phase velocity for the true solution and that of the numerical solution on $(0, \pi]$.

0.4.1 Traditional schemes

The figures show the phase velocity curves as a function of normalized wavenumber for traditional schemes, with four different γ's. For each γ, we draw the curves for four different spatial sampling rate.   From the figures we see that for all the different CFL numbers, the numerical velocity is always no bigger than the true phase velocity. So when we compute the wave equation with these schemes, we will always see wave falling behind the true wave. As the wavenumber goes up to π, the phase curve gets further less than the true dispersion curve.

First we obtain coefficients and max error with $M = 2$. (Phase velocity is the green curve in Figure 6)
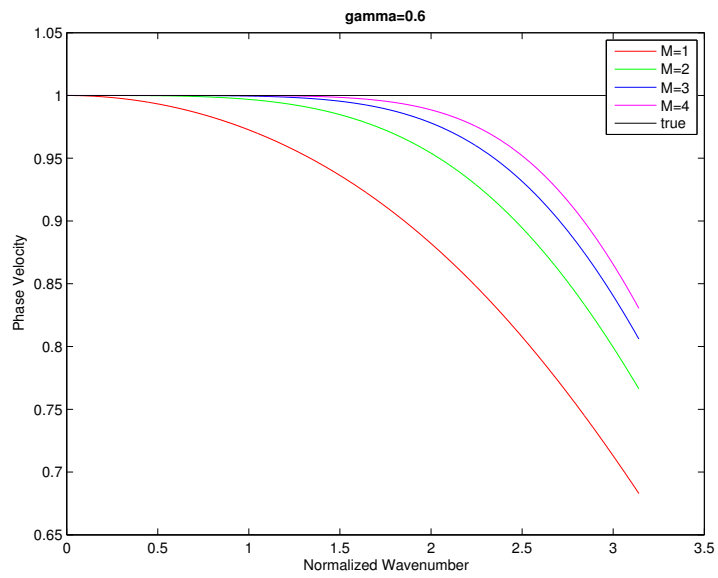
Figure 6: Velocity curves, $\gamma = 0.6$ Traditional scheme
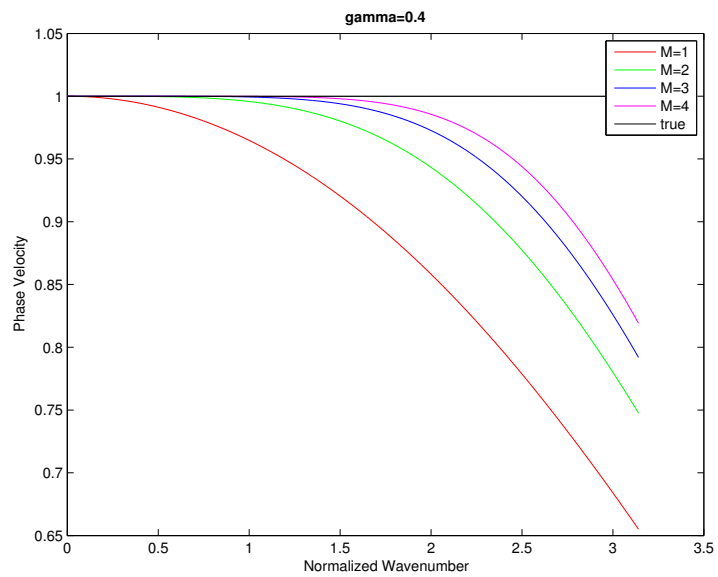
Figure 7: Velocity curves, $\gamma = 0.4$ Traditional scheme
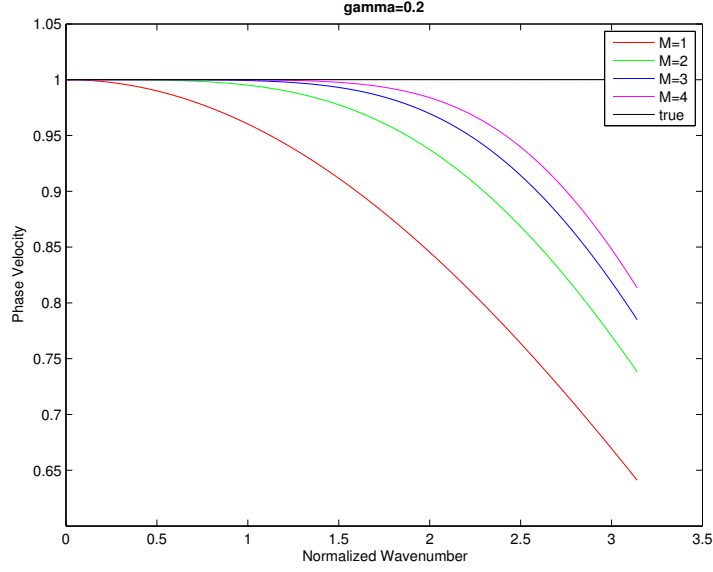
Figure 8: Velocity curves, $\gamma = 0.2$ Traditional scheme

c_0 =-0.5824, c_1 =-0.4368, c_2=0.0192

e_traditional = 0.2338

The following figures show the lagging of numerical wave at different time steps:

As we can see, after only 34 time steps, the computed wave is already behind the true wave (Figure 10); after 83 time steps, we can see that the numerical solution is roughly 1/4 wavelength behind the true solution (Figure 11). After 193 steps, we can see a slow down of half a wavelength (Figure 12).

Now we get our coefficients with $M = 3$. (Phase velocity is the blue curve in Figure 6)

c_0 =-0.5591, c_1 =-0.4717, c_2=0.0332,c_3=-0.0023

e_traditional = 0.1940

We observe a reduction of max dispersion error, as indicated in the phase velocity curve.

As we can see from Figures 13 to 16, the lagging of numerical solution is not as obvious as $M = 2$ case; as time goes on, however, lagging still occurs.
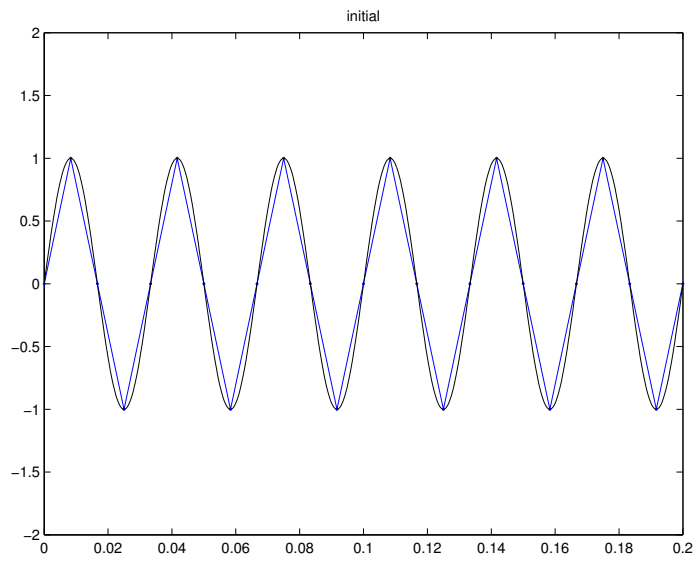
Figure 9: Initial time, traditional scheme with $M = 2$
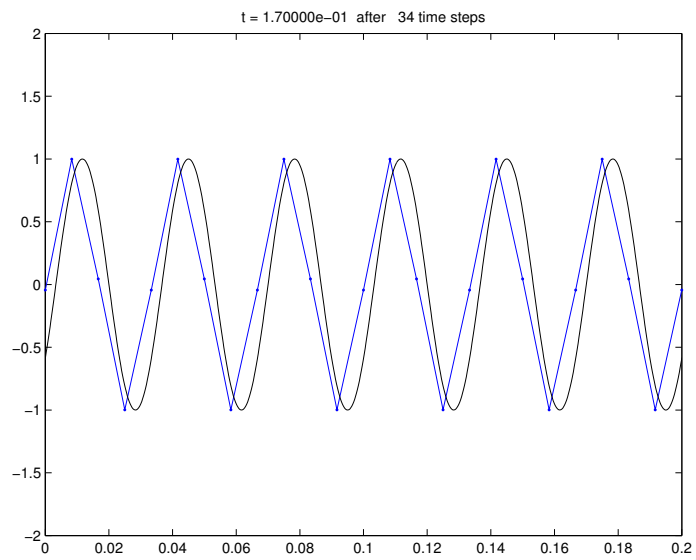
Figure 10: Time step 34, traditional scheme with $M = 2$
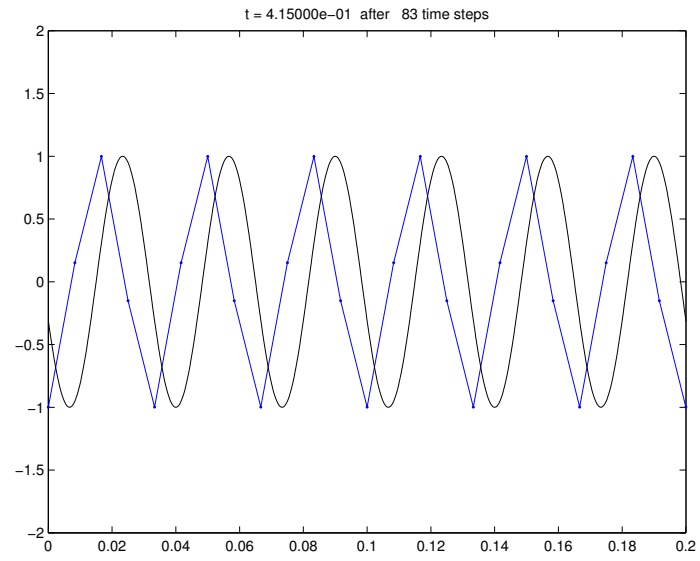
Figure 11: Time step 83, traditional scheme with $M = 2$
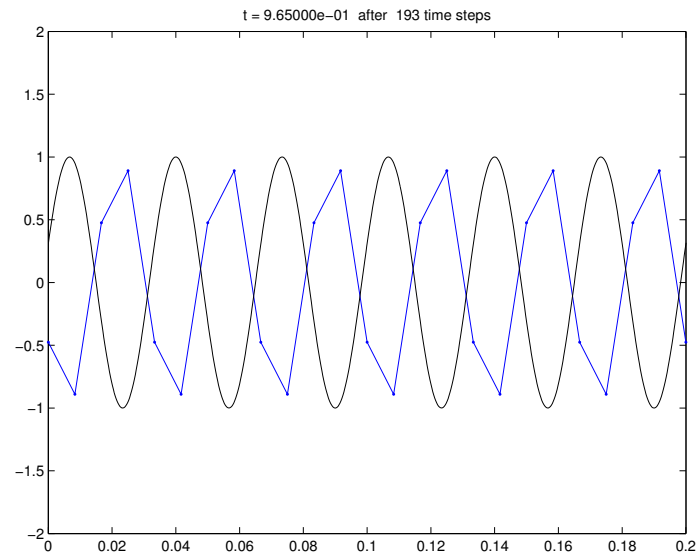
Figure 12: Time step 193, traditional scheme with $M = 2$
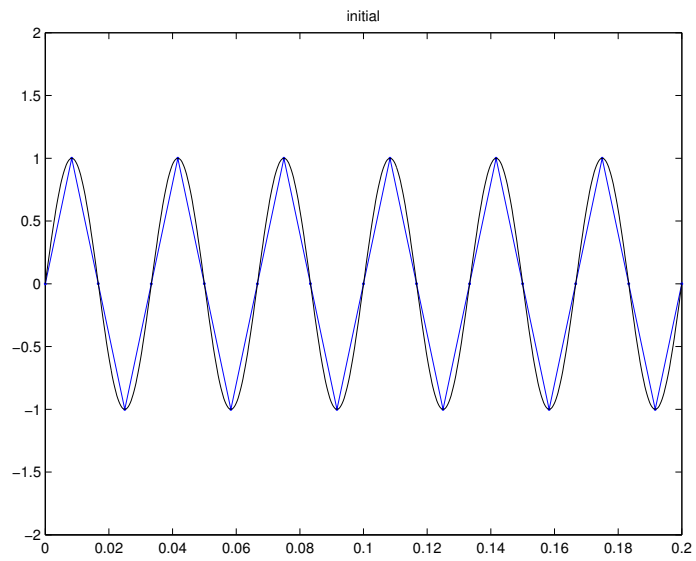
Figure 13: Initial time, traditional scheme with $M = 3$
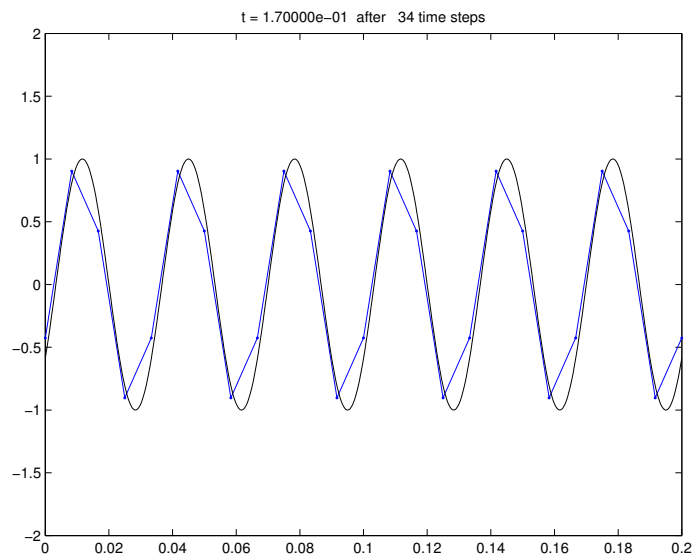
Figure 14: Time step 34, traditional scheme with $M = 3$
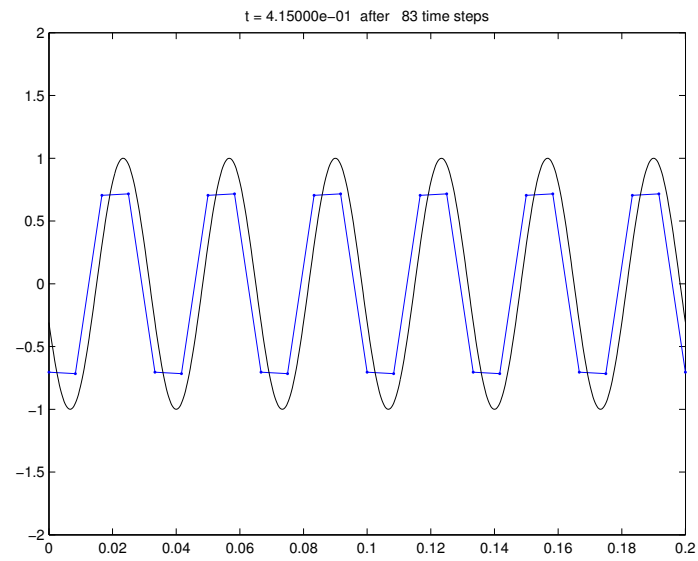
Figure 15: Time step 83, traditional scheme with $M = 3$
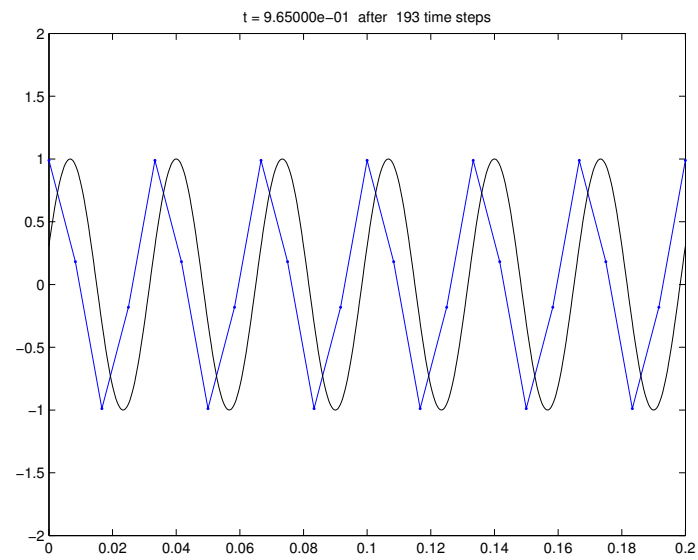
Figure 16: Time step 193, traditional scheme with $M = 3$
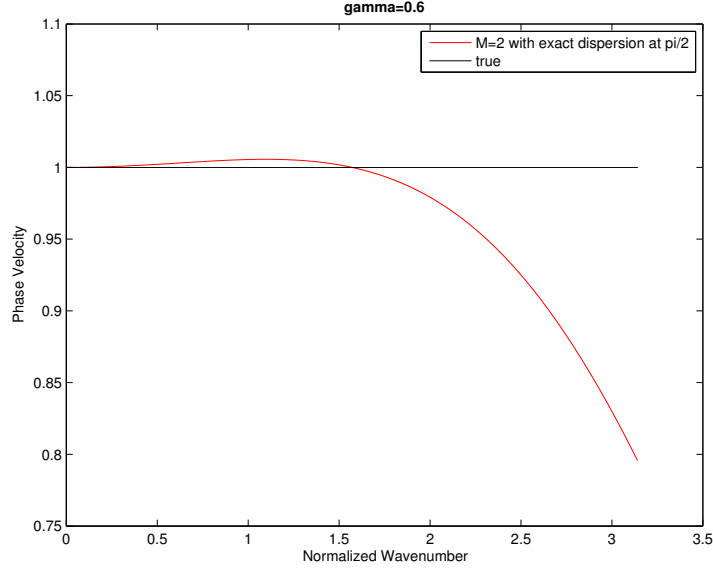
Figure 17: Velocity curve, exact dispersion at $\frac{\pi}{2}$

0.4.2 Phase velocity exact at $\frac{\pi}{2}$

For one exact dispersion, we develop scheme with $M = 2$, and assign exact dispersion at $\frac{\pi}{2}$. Phase velocity curve is drawn.

From Figure 18, we see exact phase velocity at $\frac{\pi}{2}$.

We compute the new coefficients and the max error e_new_pi_over_2 for the new scheme

```
c_0 =-0.5617, c_1 =-0.4644, c_2 =0.0261
e_new_pi_over_2 = 0.2043
```

We can see improved max error over the whole interval up to π compared with traditional $M = 2$ scheme.

We can see obvious improvement for the numerical phase velocity compared to the traditional method from Figures 20 to 22. After 865 time steps, we still get almost the same velocity for the numerical and true solution.
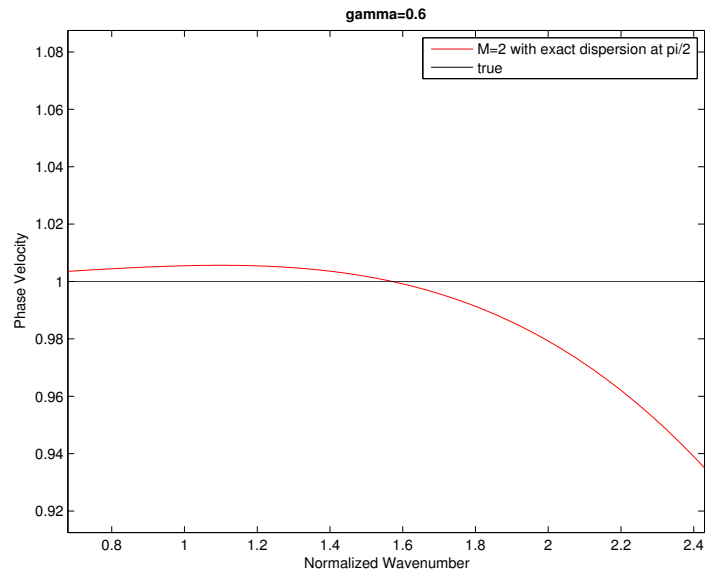
Figure 18: Velocity curve, exact dispersion at $\frac{\pi}{2}$, blow-up
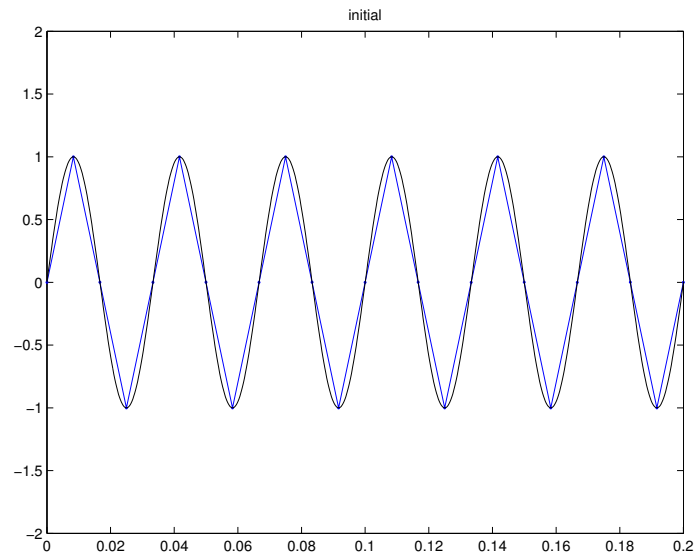
Figure 19: Initial time, Exact dispersion at $\frac{\pi}{2}$, with $M = 2$
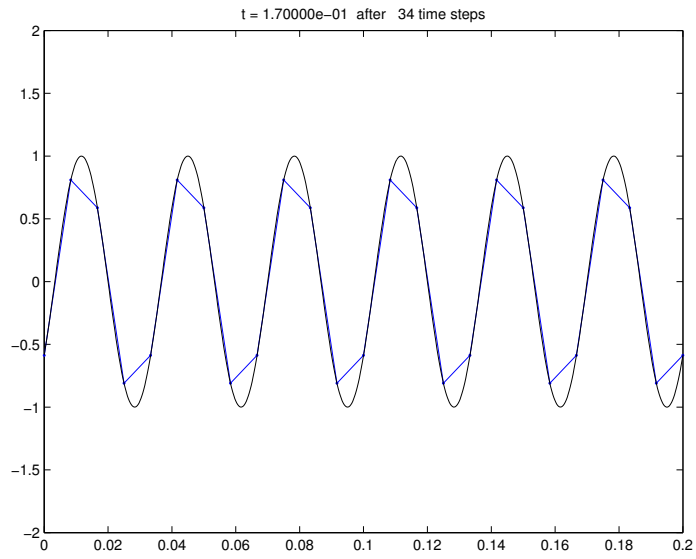
Figure 20: Time step 34, Exact dispersion at $\frac{\pi}{2}$, with $M = 2$
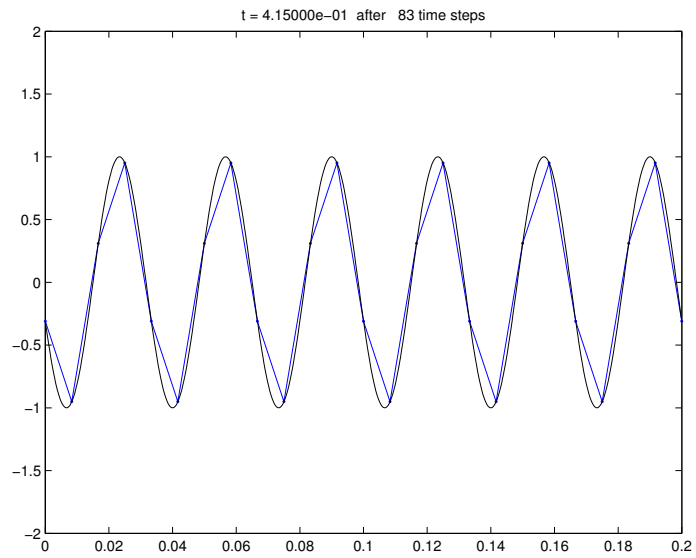
Figure 21: Time step 83, Exact dispersion at $\frac{\pi}{2}$, with $M = 2$

t = 4.32500e+00 after 865 time steps
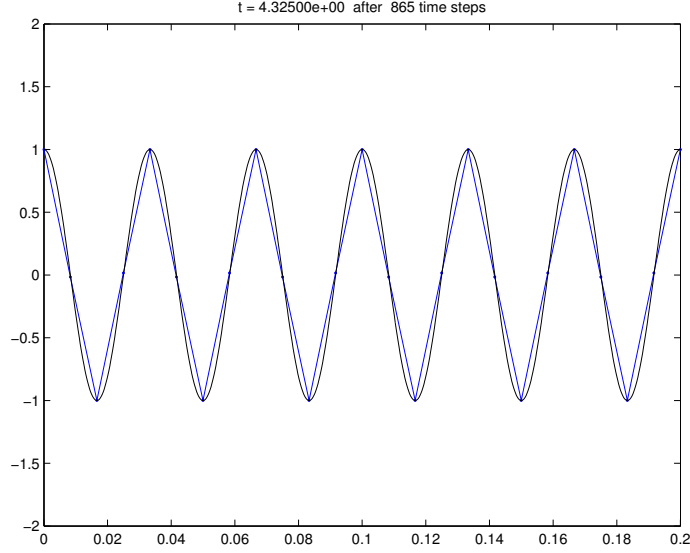
Figure 22: Time step 865, Exact dispersion at $\frac{\pi}{2}$, with $M = 2$

0.4.3   Phase velocity exact at $K_1 = \frac{\pi}{2}$ and $K_2 = \frac{\pi}{2} + \frac{\pi}{8}$

Now we examine the new schemes with two exact dispersion assigned. In this section, we will look at the case for $M = 3$ for all wave propagation experiments. First we show figures of dispersion curve with exact dispersion at $\frac{\pi}{2}$ and another wavenumber near by. Coefficients are obtained with $K_1 = \frac{\pi}{2}$ and $K_2 = \frac{\pi}{2} + \frac{\pi}{8}$. We first show dispersion curves.

```
c_0 =-0.5347, c_1 =-0.5116, c_2 =0.0531, c_3=-0.0067
e_new_pi_2_twopoints = 0.1470
```

There is an observed improvement of overall approximation to dispersion from above computation.

Now we use the new set of coefficients to compute the wave propagation

After 865 time steps, there is still no obvious phase lag, as expected.
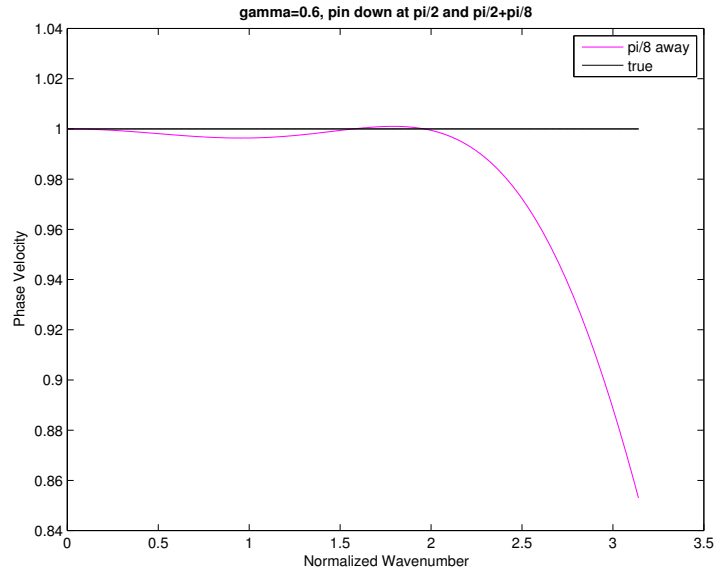
Figure 23: Velocity curve, exact dispersion at $\frac{\pi}{2}$ and $\frac{\pi}{2} + \frac{\pi}{8}$ $M = 3$
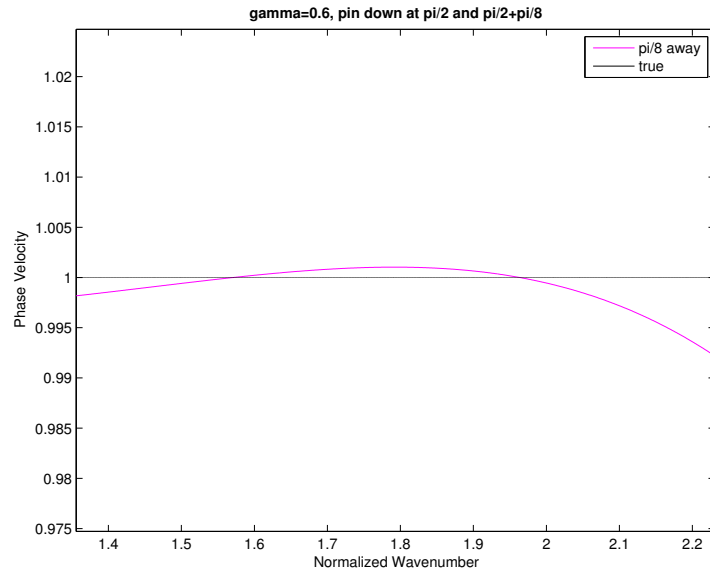

Figure 24: Velocity curve, exact dispersion at $\frac{\pi}{2}$ and $\frac{\pi}{2} + \frac{\pi}{8}$, $M = 3$, blow-up
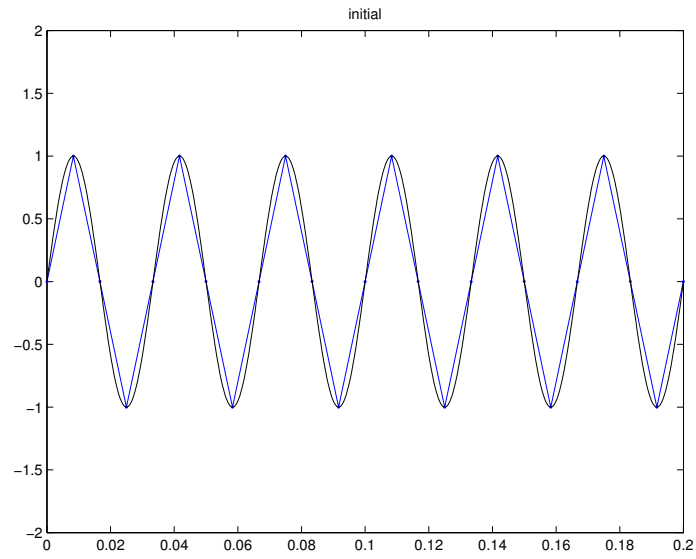
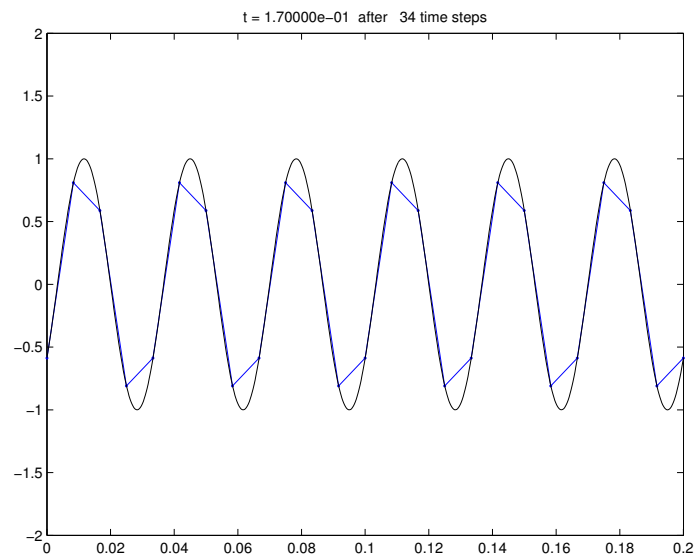Figure 25: Initial time, exact dispersion at $\frac{\pi}{2}$ and $\frac{\pi}{2} + \frac{\pi}{8}$, $M = 3$

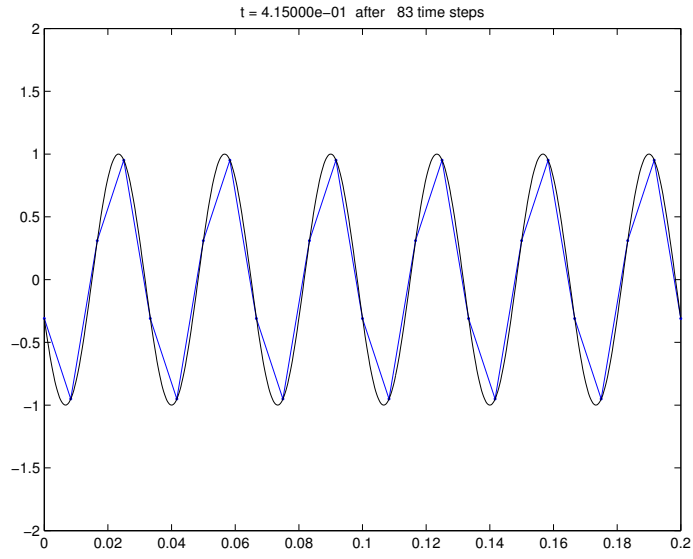Figure 26: Time step 34, exact dispersion at $\frac{\pi}{2}$ and $\frac{\pi}{2} + \frac{\pi}{8}$, $M = 3$

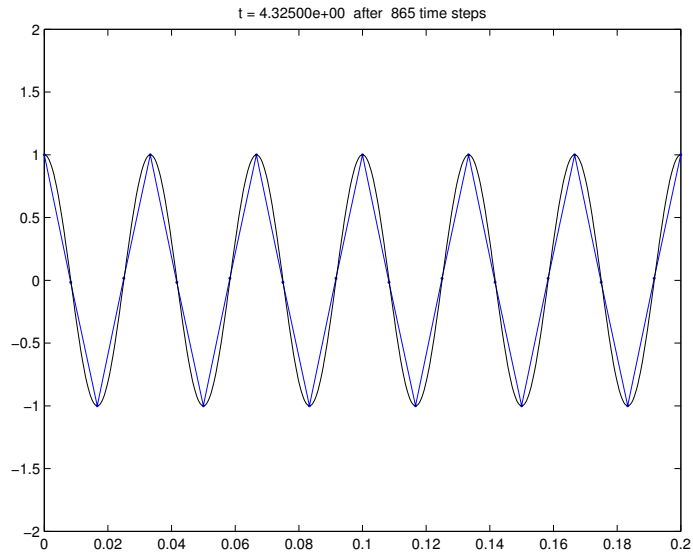Figure 27: Time step 83, exact dispersion at $\frac{\pi}{2}$ and $\frac{\pi}{2} + \frac{\pi}{8}$, $M = 3$

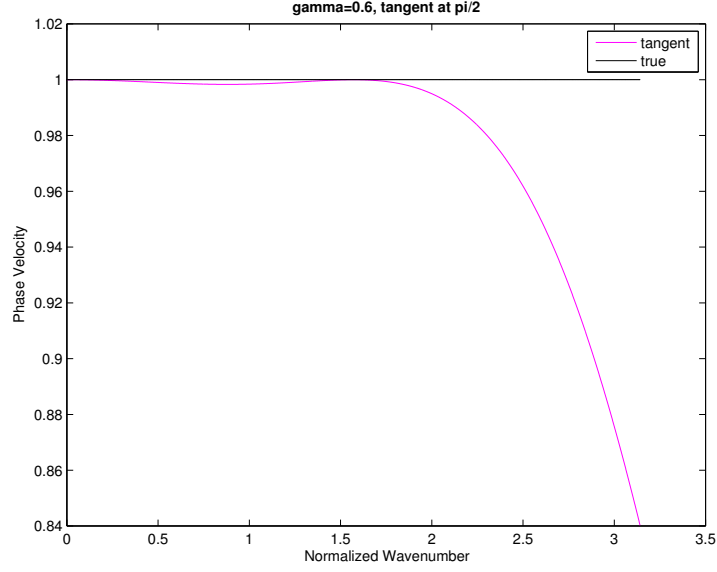Figure 28: Time step 865, exact dispersion at $\frac{\pi}{2}$ and $\frac{\pi}{2} + \frac{\pi}{8}$, $M = 3$

Figure 29: Velocity curve, tangent approximation, $M = 3$

0.4.4 Higher order approximation of phase velocity at $\frac{\pi}{2}$

Here we present the scheme discussed in Section 3.3.

```
c_0 =-0.5407, c_1 =-0.5011, c_2 =0.0471, c_3=-0.0052
e_new_pi_over_2_tangent = 0.1597
```

The phase velocity curve are drawn in Figure 29 and 30. Tangent approximation at $\frac{\pi}{2}$ can be easily seen.

Now we use the coefficients above to compute wave propagation. As shown below (Figure 34), we ger really good approximation at time step 865.

Finally we show the dispersion curves drawn with two points pinned down and higher order approximation, for four different CFL numbers γ. The legends indicate how far the second point is from $\frac{\pi}{2}$. (Figures 35 to 38)
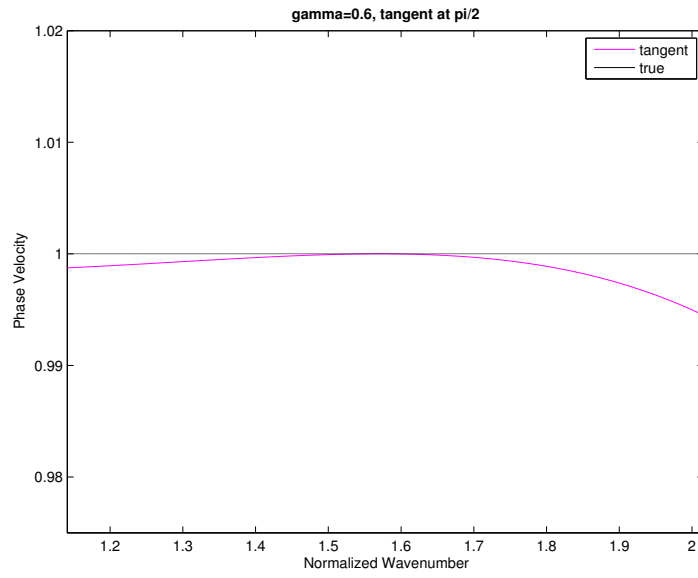
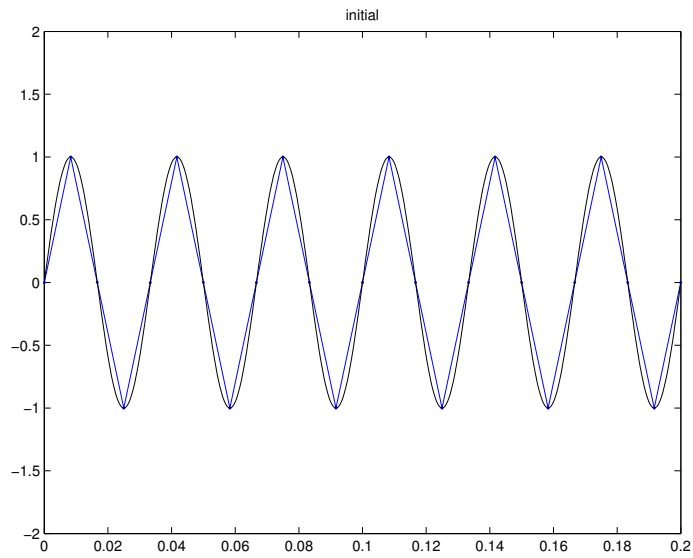Figure 30: Velocity curve, tangent approximation, $M = 3$, blow-up

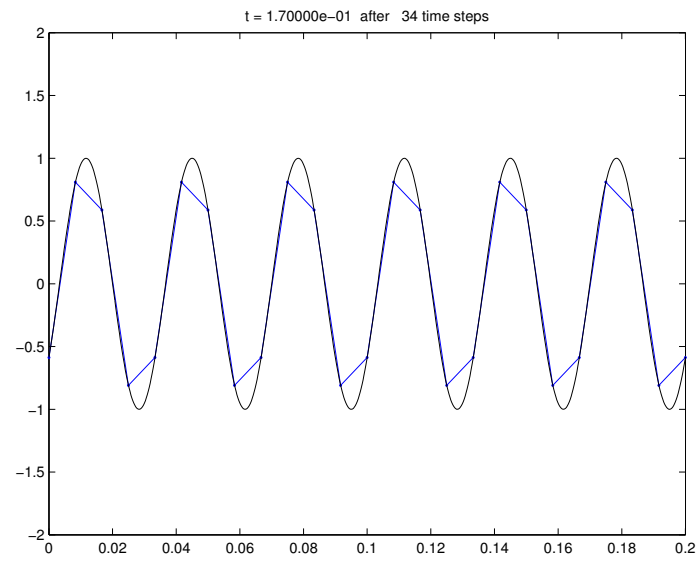Figure 31: Initial time, with tangent approximation, $M = 3$

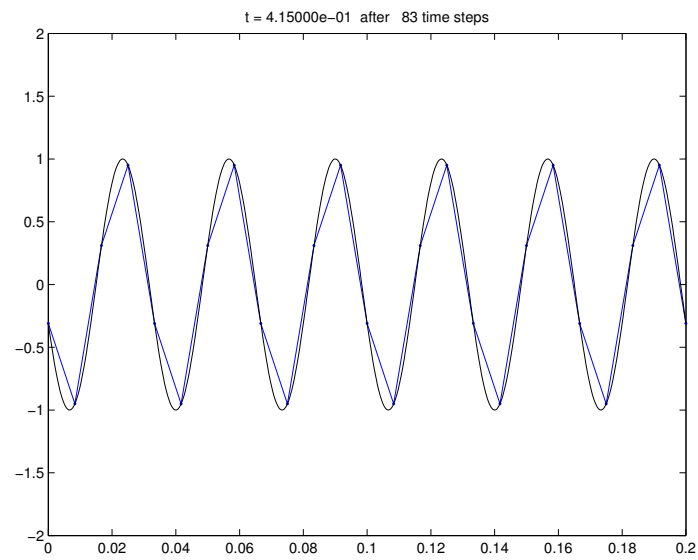Figure 32: Time step 34, with tangent approximation, $M = 3$

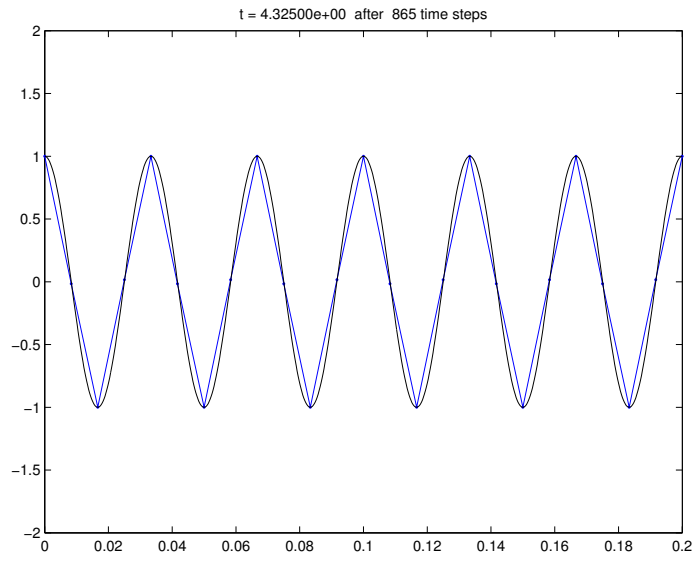Figure 33: Time step 83, with tangent approximation, $M = 3$

Figure 34: Time step 865, with tangent approximation, $M = 3$
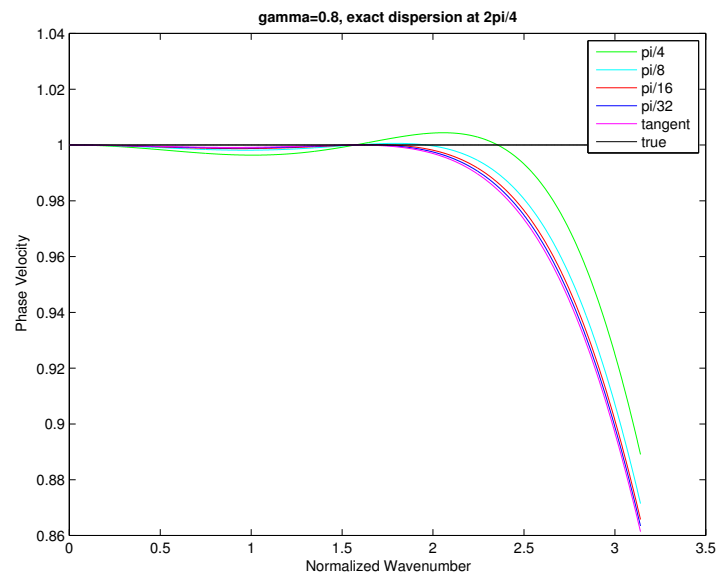

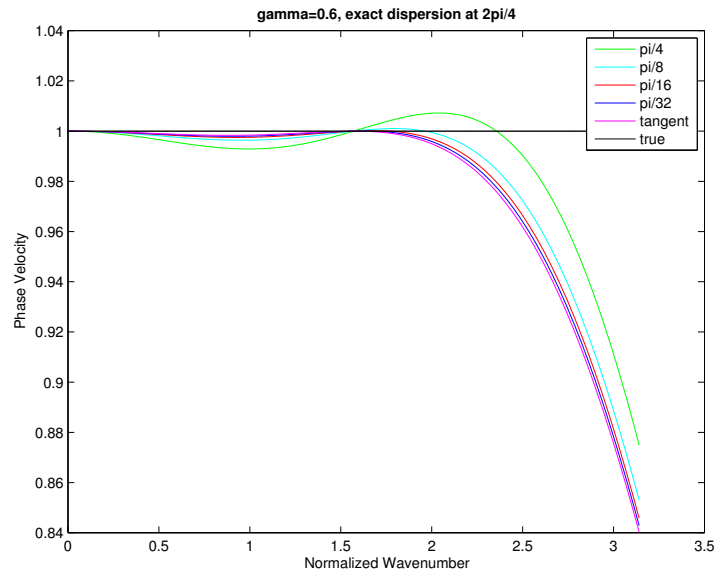Figure 35: Velocity curve, $\gamma = 0.8$
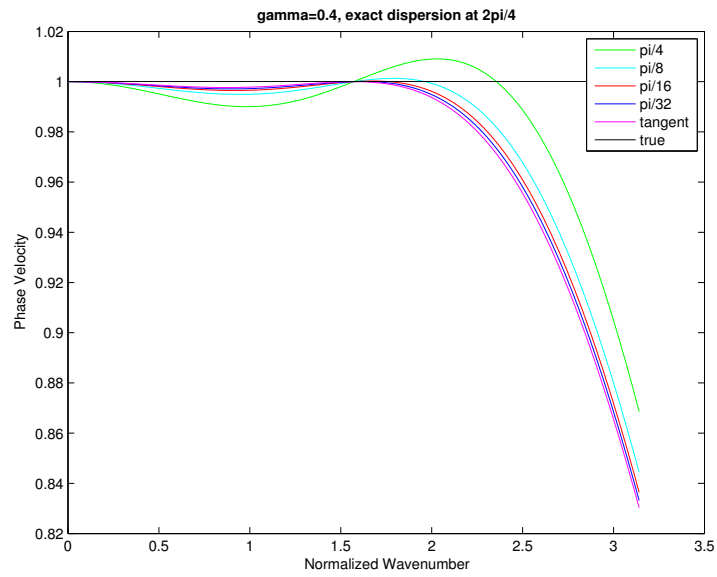
Figure 36: Velocity curve, $\gamma = 0.6$

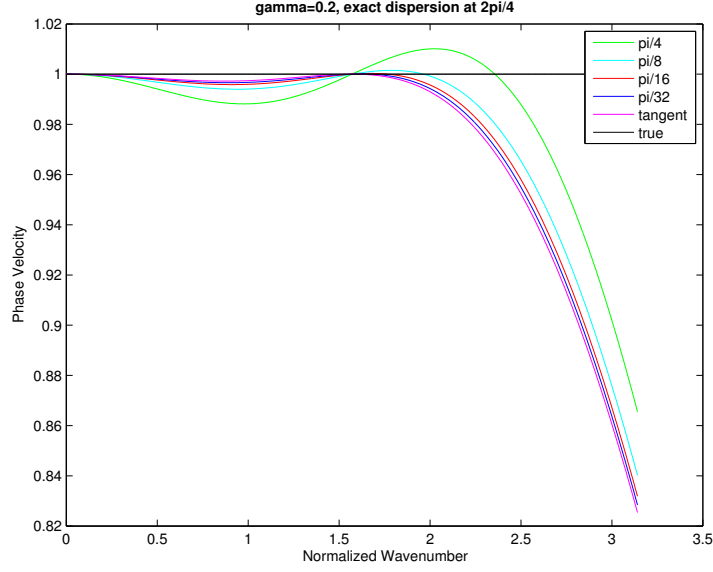Figure 37: Velocity curve, $\gamma = 0.4$

Figure 38: Velocity curve, $\gamma = 0.2$

0.5 2D and higher dimension cases

For higher dimension cases, we consider the equation $\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0$. In two dimensional case for example, we start off with the following discretization [5]

$$u_{i,j}^{n+1} - 2u_{i,j}^n + u_{i,j}^{n-1} - \gamma_x^2 \left[u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n \right] - \gamma_y^2 \left[u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n \right] = 0$$

with $\gamma_x = \frac{c\Delta t}{\Delta x}$ and $\gamma_y = \frac{c\Delta t}{\Delta y}$. Group the symmetric terms and free the coefficients to obtain a general scheme

$$u_{i,j}^{n+1} + u_{i,j}^{n-1} - 2c_1 u_{i,j}^n + c_2(u_{i+1,j}^n + u_{i-1,j}^n) + c_3(u_{i,j+1}^n + u_{i,j-1}^n) = 0$$

Do discrete Fourier transform to obain our dispersion relation

$$\cos(\Omega) + c_1 + c_2 \cos(K_x) + c_3 \cos(K_y) = 0$$

Here $K_x = \xi_x \Delta x$ and $K_y = \xi_y \Delta y$ denotes respectively the x and y direction in spectral domain. We can choose to solve for new scheme only concerning ourselves with these two directions, which uses essentially the same strategy as the one-dimensional case; A more interesting point of view is to replace K_x and K_y with spectral direction depending terms $K \cos(\phi)$ and $K \sin(\phi)$, thus obtain the dispersion relation

$$\cos(\Omega) + c_1 + c_2 \cos(K \cos(\phi)) + c_3 \cos(K \sin(\phi)) = 0$$

Now we have more freedom to choose how to obtain the scheme. For example, here we can fix one angle ϕ and pick three different wavenumbers for the dispersion to be exact; we can look at three different angles, but at only one wavenumber; or we pick three pairs of (ϕ, K).

If we apply the same stencil in both x and y direction, and set up our general scheme as

$$u_{i,j}^{n+1} + u_{i,j}^{n-1} + \sum_{m=0}^{M} c_m (u_{i+m,j}^n + u_{i-m,j}^n + u_{i,j+m}^n + u_{i,j-m}^n) = 0$$

discrete Fourier transform gives the following numerical dispersion

$$\cos(\Omega) + \sum_{m=0}^{M} c_m [\cos(mK \cos(\phi)) + \cos(mK \sin(\phi))] = 0$$

We apply the same analysis as in Section 3 to do Taylor expansion at $(\Omega, K) = (0, 0)$ with accuracy requirements

$$\gamma^{2j} + \sum_{m=0}^{M} c_m m^{2j} [\cos(\phi)^{2j} + \sin(\phi)^{2j}] = 0 \ j = 0, \ldots, p$$

Now the coefficients for our scheme are angle dependent. Let $f_j(\phi) = \cos(\phi)^{2j} + \sin(\phi)^{2j}$. Liu and Sen in their work [11] found the angle $\frac{\pi}{8}$ as their optimal choice, for $f_j(\frac{\pi}{8})$ gives the most repeat values for ϕ within $[-\pi, \pi]$. This can be easily seen as

$$f_j(\phi) = \cos(\phi)^{2j} + \sin(\phi)^{2j} = \frac{1}{2^j}(1 - \cos(2\phi))^j + \frac{1}{2^j}(1 + \cos(2\phi))^j$$

The fact that $\cos(2\phi)$ is even function itself, and both of $\cos(2\phi)$, $-\cos(2\phi)$ are in the function indicates that we can find 8 repeats when taking ϕ between 0 and $\frac{\pi}{4}$, $\frac{\pi}{8}$ being the middle guarantees even distribution of angles.

One of our future goals is to look at angle dependence and solve for the coefficients such that we get a good approximation uniformly in angle. For the 3-dimensional problem, Wang and Teixeira [15] first expanded the numerical dispersion error (same as our ϵ in Section 2) in spherical harmonics in terms of propagating angle, then made the first few terms made to be zero. Now the scheme is frequency dependent, they then do Taylor expansion in the frequency variable.

0.6 Group velocity

For dispersive equations, problems concerning speed of propagation arise when we are dealing with a wave packet containing several modes with different frequencies. Consider an initial wave packet $f(x,0)$ near the origin, with Fourier transform $\hat{f}(\xi)$, then at time $t \geq 0$, the solution is

$$f(x,t) = \int_{-\infty}^{\infty} \hat{f}(\xi) e^{i(\omega(\xi)t - \xi x)} d\xi$$

Now this solution is a superposition of waves of different wavenumbers, each traveling with its own phase velocity $c_p(\xi)$, dispersing as time evolves. As $t \to \infty$, we can only observe wave at stationary phase with respect to ξ, i.e. $\frac{d}{d\xi}\left(\omega(\xi) - \frac{\xi x}{t}\right) = 0$, $\frac{d\omega}{d\xi} - \frac{x}{t} = 0$. We define

$$c_g(\xi) = \frac{d\omega(\xi)}{d\xi}$$

to be the *group velocity* [16]. Group velocity carries information about energy of the wave packet, so we will develop schemes in the future aiming at giving good approximation of group velocity.

Generally, phase velocity and group velocity are not equal. For example, for dispersive equation

$$u_t + a u_x + b u_{xxx} = 0$$

with dispersion relation $\omega(\xi) = a\xi - b\xi^2$, then we have

$$c_g(\xi) = a - 3b\xi^2$$

but

$$c_p(\xi) = a - b\xi^2$$

Now we look at the numerical group velocity computed from three common schemes. Use the fact $\frac{d\omega}{d\xi} = 1$, we implicitly differentiate the above equations with respect to ξ to get

$$\text{LF } \sin(\omega\Delta t) = \frac{\Delta t}{\Delta x}\sin(\xi\Delta x)$$

$$\text{CN } 2\tan(\frac{\omega\Delta t}{2})\sec^2(\frac{\omega\Delta t}{2}) = \frac{\Delta t}{\Delta x}\sin(\xi\Delta x)$$

$$\text{LF4 } \sin(\omega\Delta t) = \frac{4}{3}\frac{\Delta t}{\Delta x}\sin(\xi\Delta x) - \frac{1}{6}\frac{\Delta t}{\Delta x}\sin(2\xi\Delta x)$$

Note that the Nyquist frequency gives zero group velocity and in this sense, we treat Nyquist as a singularity for this computation, we will have to make a choice between good approximation and information on the whole spectral domain. We would like to find a theorical upper bound of wavenumbers, and develop schemes that give 'good' numerical group velocity for all wavenumbers up to that upper bound.

Here we show wave propagation with initial wave packet $u(x,0) = e^{-16(x-0.5)^2}\sin(2\pi\xi x)$. Figure 39 is drawn with traditional scheme for $M = 2$, and Figure 40 with the new scheme developed with exact dispersion at $K = \frac{\pi}{2}$. Take $\gamma = 0.6$.

As we can see, using scheme developed for exact phase velocity still helps reduce the lag in group velocity. We would like to study schemes improving group velocity dispersion directly.
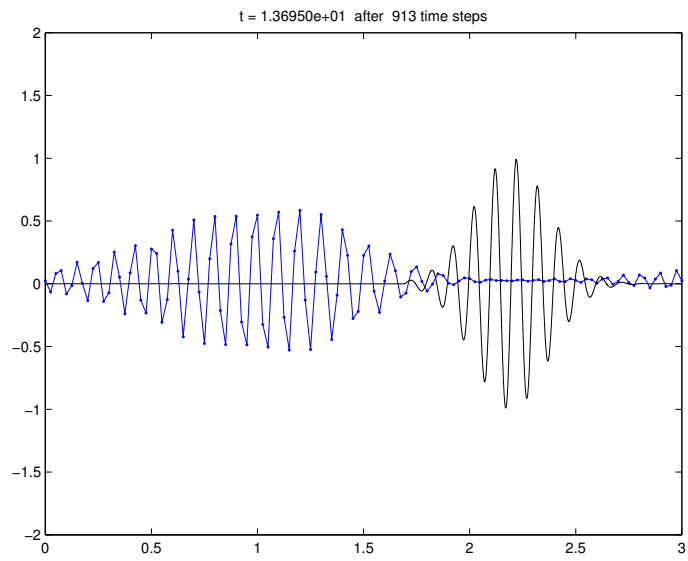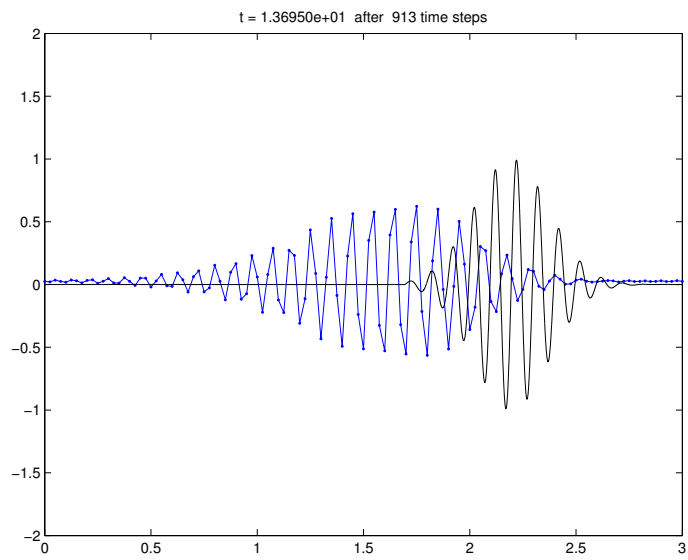
Figure 39: Traditional scheme, $M = 2$, wave packet

Figure 40: New scheme, $M = 2$, wave packet

0.7 Appendix: MATLAB code

The following code is used to compute the wave equation with the (3,5) stencil, both put all constraints on accuracy at zero, and assign exact dispersion at one frequcies.

```
% solve the wave equation with c=1
function []=wave_29(n)

global c
c = 1;
L=3;

dx=L/(n+1); % need mod(n+1,4L)=0. L=3 implies (n+1)/12=integer
xi = 2*pi/(4*dx*2*pi); %xi has to be integer.
%%%%%%%%%%%%%%%%%
dt=0.6*dx;

stoptime=1000;
%r=c*dt/dx;
xfine = 0:0.0001*L:L;

past=utrue(0:dx:L,0,xi);
past(1)=past(n+2);
past(n+3)=past(2);
past(n+4)=past(3);
past(n+5)=past(4);
%%%%%%%%%%%%%%%%%%%%%%%%%%%
ufinepast = utrue(xfine,0,xi);
        plot(0:dx:L,past(1:n+2),'b.-',xfine,ufinepast,'k')
```

```
%plot(0:dx:L,past(1:n+2))
axis([0 L -2 2])
pause


%%%%%%%%%%%%%%%%%%%%%%%%%


current=utrue(0:dx:L,dt,xi);
current(1)=current(n+2);
current(n+3)=current(2);
current(n+4)=current(3);
current(n+5)=current(4);
%%%%%%%%%%%%%%%%%%%%%%%%%%%
ufinenow = utrue(xfine,dt,xi);
        plot(0:dx:L,current(1:n+2),'b.-',xfine,ufinenow,'k')
%plot(0:dx:L,current(1:n+2))
axis([0 L -2 2])
pause


%%%%%%%%%%%%%%%%%%%%%%%%%%%
%c0=-0.5824;c1=-0.4368;c2= 0.0192; % only accuracy at zero.
c0=-0.5617;c1=-0.4644;c2= 0.0261; % exact dispersion at K0=pi/2; pair with
%n=359


%%%%%%%%%%%%%%%%%%%%%%%%%%%%


for t=2*dt:dt:stoptime
```

```
        future(3:n+3)=-2*c0*current(3:n+3)-past(3:n+3)-c1*(current(4:n+4)+...
        current(2:n+2))-c2*(current(5:n+5)+current(1:n+1));


        future(1)=future(n+2);
        future(2)=future(n+3);
        future(n+4)=future(3);
        future(n+5)=future(4);




        past=current;
        current=future;
         % if mod(t/dt,10000)==0
            ufine = utrue(xfine,t,xi);
            plot(0:dx:L,current(1:n+2),'b.-',xfine,ufine,'k')
            title(sprintf('t = %9.5e  after %4i time steps',...
                        t,t/dt))
            axis([0 L -2 2])



            pause%(0.01)


        % end
    end


function utrue = utrue(x,t,xi)
% true solution for comparison
```

```matlab
global c

% For periodic BC's, we need the periodic extension of eta(x,xi).
% Map x-a*t back to unit interval:

xat = rem(x - c*t, 3);
ineg = find(xat<0);
xat(ineg) = xat(ineg) + 3;
utrue = eta(xat,xi);
return


%------------------------------------------------------------

function eta = eta(x,xi)
% initial data

beta = 16;

eta = sin(2*pi*xi*x);%need to make xi integer for pbc
return
```

0.8 References

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