Turkish Journal of Mathematics

http://journals.tubitak.gov.tr/math/

Research Article

Turk J Math
(2016) 40: 806 – 815

doi:10.3906/mat-1506-24

Simulations of the Helmholtz equation at any wave number for adaptive grids using a modified central finite difference scheme

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Received: 08.06.2015 • **Accepted/Published Online:** 27.10.2015 • **Final Version:** 16.06.2016

Abstract: In this paper, a modified central finite difference scheme for a three-point nonuniform grid is presented for the one-dimensional homogeneous Helmholtz equation using the Bloch wave property. The modified scheme provides highly accurate solutions at the nodes of the nonuniform grid for very small to very large range of wave numbers irrespective of how the grid is adapted throughout the domain. A variety of numerical examples are considered to validate the superiority of the modified scheme for a nonuniform grid over a standard central finite difference scheme.

Key words: Helmholtz equation, modified central finite difference scheme, numerical dispersion, nonuniform grids, adaptive grids

1. Introduction

Numerical dispersion has always been a hindrance for the accurate simulations of the Helmholtz equation and to reduce or eliminate it one needs to use extremely refined mesh, resulting in prohibitive computational cost. Reducing numerical dispersion really becomes untractable (a) in the case of large wave numbers because of the highly oscillatory behavior of waves; (b) when the problem is posed in higher dimensions because of anisotropy; (c) when the discretization of the domain is not uniform. Many efforts have already been made in the last few decades to solve the Helmholtz equation [1–4, 9, 10, 19] and it is not surprising that finite difference methods have been the choice of many [11, 13, 16–18] for the accurate simulations of the Helmholtz equation. However, the surprising thing is that all of these efforts were just devoted to the construction of schemes on uniform discretization of the domain [11, 13, 16–18]. No real effort is evident in the case of nonuniform discretization as it is widely known that in the case of nonuniform grids the order of accuracy of the derivative approximation generally is less than that of uniform grids [7, 15]. Consequently, because of the lack of symmetry of nonuniform grids the standard central finite difference schemes provide less accurate results for the Helmholtz equation.

Relatively recently, in [14, 24] efforts were made to construct schemes for the homogeneous Helmholtz equation that provide pollution-free solutions at the nodes of a uniform grid for any range of wave number by modifying the standard central finite difference approximations. Later on, in [22] this was further extended to construct pollution-free finite difference schemes for the nonhomogeneous Helmholtz equation. Moreover, details about constructing exact finite difference solutions in the case of polar and spherical coordinates can be found in [23]. Furthermore, in [5], the use of the method of difference potential for the computation of singular

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solutions of the Helmholtz equation with higher order of accuracy is presented in detail. However, numerical simulations of the acoustic wave equation with reduced grid dispersion effects were proposed in [12] that satisfy the dispersion relation for a number of uniformly distributed wavenumber points within a wavenumber domain with the upper limit determined by the maximum source frequency, the grid spacing, and the wave velocity. Moreover, in [12] it was shown that this new dispersion relationship preserving method relatively uniformly reduces the numerical dispersion over a large frequency range.

In [21], modified forward, backward, and central finite difference schemes were constructed, specifically for the homogeneous Helmholtz equation, by using the Bloch wave property. It was shown in [21] that all of these modified finite difference approximations provide exact solutions at the nodes of the uniform grid for the second derivative present in the Helmholtz equation and the first derivative in the radiation boundary conditions for wave propagation. In the present paper, we focus on constructing pollution-free central finite difference approximations for the one-dimensional homogeneous Helmholtz equation in the case of a nonuniform grid using the Bloch wave property.

The organization of the paper is as follows. Section 2 presents standard central finite difference schemes for uniform and three-point nonuniform grids. Afterwards, in Section 3 a framework for a modified central finite difference scheme is presented. In Section 4, the cheap implementation of modified schemes is described. Finally, numerical examples along with graphical analysis are given in detail in Section 5, followed by a few remarks.

2. Standard central finite difference (CFD) schemes for uniform and nonuniform grids

In order to motivate the ideas, we consider the one-dimensional Helmholtz equation [8]

$$u''(x) + k^2 u(x) = 0 \qquad \text{for } x \in \mathbb{R} \tag{2.1}$$

where $k \in \mathbb{C}$ is the wave number. We now discretize domain $\mathbb{R}$ such that before and after the node x_j, we have uniformly spaced grids, meaning that we have a three-point nonuniform grid denoted by $G_j = \{x_{j-1}, x_j, x_{j+1}\}$, such that $x_j - x_{j-1} = h_1$ and $x_{j+1} - x_j = h_2$ with $h_1 - h_2 \neq 0$ and $h_1, h_2 > 0$. For a nonuniform grid the discrete approximation of the second derivative present in the Helmholtz equation 2.1 is given by [15]

$$\begin{aligned} u_j'' &= \frac{2}{h_1(h_1+h_2)} u_{j-1} - \frac{2}{h_1 h_2} u_j + \frac{2}{h_2(h_1+h_2)} u_{j+1} \\ &- \frac{h_2 - h_1}{3} u_j^{(3)} - \frac{h_1^2 - h_1 h_2 + h_2^2}{12} u_j^{(4)} + \cdots \end{aligned} \tag{2.2}$$

which is first-order accurate in comparison to the case of a uniform grid i.e. $h_1 = h_2 = h$ given by [20]

$$u_j'' = \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} - \frac{h^2}{12} u_j^{(4)} + \cdots \tag{2.3}$$

which is second-order accurate. Hence, the order of accuracy of the derivatives' approximations for nonuniform grids is in general less than that of uniform grids and the reason for this is the lack of symmetry in the case of nonuniform grids [15]. Inserting 2.2 into 2.1, we obtain the following stencil

$$2h_2 u_{j-1} + (h_1 + h_2)(h_1 h_2 k^2 - 2) u_j + 2h_1 u_{j+1} = 0 \tag{2.4}$$

which leads back to

$$u_{j-1}+(h^2k^2-2)u_j+u_{j+1}=0 \tag{2.5}$$

for $h_1=h_2=h$. The finite difference approximation 2.4 of the Helmholtz equation for nonuniform grids is also given in [17]. It is very well known [1, 3, 6, 8, 19] in the case of scheme 2.5 that relative numerical dispersion error is given by

$$\left|\frac{k-\tilde{k}}{\tilde{k}}\right|=\frac{(\tilde{k}h)^2}{24}+\mathcal{O}((\tilde{k}h)^4) \tag{2.6}$$

with $\tilde{k}$ as the discrete wave number. Now, in order to measure numerical dispersion for modified scheme 2.4, we insert plane wave solutions of the forms $u_j=e^{ij\tilde{k}h_1}$ and $u_j=e^{ij\tilde{k}h_2}$ for regions before and after node x_j with grid spacings $h_1>0$ and $h_2>0$ respectively and solving for k we get

$$k=\frac{\sqrt{2h_1h_2(h_1+h_2)\left(h_1+h_2-h_1e^{i\tilde{k}h_2}-h_2e^{i\tilde{k}h_1}\right)}}{h_1h_2(h_1+h_2)}.$$

Rewriting the above expression as a series, we get the relative numerical dispersion error given by

$$\left|\frac{k-\tilde{k}}{\tilde{k}}\right|=\frac{\tilde{k}}{72}\left|12(h_1-h_2)I+\tilde{k}\left(2h_1^2-h_1h_2+2h_2^2\right)\right|+\mathcal{O}((\tilde{k}h_1)^3)+\mathcal{O}((\tilde{k}h_2)^3) \tag{2.7}$$

which results in 2.6 for $h_1=h_2=h$.

It is evident from 2.6 and 2.7 that to obtain dispersion-free propagation both for uniform and nonuniform grids requires exact and discrete wave numbers to be exactly the same i.e. $\tilde{k}=k$ at the nodes of uniform and nonuniform grids respectively. With this in mind, modified finite difference schemes were constructed in [21] for the case of uniform grids using the Bloch wave property. In the following sections, we present a framework for the construction of a modified CFD scheme for a three-point nonuniform grid using the Bloch wave property for the one-dimensional Helmholtz equation.

3. Framework for a modified central finite difference scheme for a nonuniform grid

For this, we consider the discrete Bloch wave property defined in [21] for uniform grids given by

$$u_{j+n}=e^{ikhn}u_j \quad \forall\, n\in\mathbb{Z},\ h>0. \tag{3.1}$$

Since we have a three-point nonuniform grid at the node x_j, and for both uniformly spaced grids with grid spacings $h_1>0$ and $h_2>0$ before and after the node x_j respectively, we have the following definitions for the Bloch wave property:

$$u_{j-n}=e^{-ikh_1n}u_j \quad \forall\, n\in\mathbb{N},\ h_1>0 \tag{3.2}$$

and

$$u_{j+m}=e^{ikh_2m}u_j \quad \forall\, m\in\mathbb{N},\ h_2>0. \tag{3.3}$$

Making use of 3.2 and 3.3 in 2.4, we obtain

$$2h_2u_{j-1}+(h_1+h_2)(h_1h_2k^2-2)u_j+2h_2u_{j+1}=(2h_2e^{-ikh_1}+2h_1e^{ikh_2}+(h_1+h_2)(h_1h_2k^2-2))u_j$$

or, rewriting

$$h_2 u_{j-1} - (h_2 e^{-ikh_1} + h_1 e^{ikh_2}) u_j + h_1 u_{j+1} = 0. \tag{3.4}$$

For $h_1 = h_2 = h$, the above equation 3.4 leads back to the following:

$$u_{j-1} - 2\cos(kh) u_j + u_{j+1} = 0 \tag{3.5}$$

obtained for the case of uniform grids in [21]. Moreover, the above scheme was also presented in texts [14, 24] with alternative formulations. However, their construction cannot easily be extended to nonuniform grids. Interestingly, the series representations of middle nodes in 3.4 and 3.5 lead back to standard schemes 2.4 and 2.5, respectively.

4. Easy implementation of the modified CFD schemes for both uniform and nonuniform grids

An interesting feature of the modified CFD schemes 3.4 and 3.5 is their easy implementation, which does not require one to write a brand new code; instead one just needs to replace the coefficient of the middle nodes in the standard CFD schemes with novel coefficients. Furthermore, 3.4 and 3.5 keep the same bandwidth structure as one has in the case of standard CFD schemes and therefore adds no additional cost to the implementation while providing highly accurate results for all ranges of wave numbers even for nonuniform grids.

Table 1. Comparison of dispersion errors for standard and modified central finite difference schemes for fixed $kh = 0.5$ with varying wave number for the case of boundary conditions 5.1 for a uniform grid and a three-point nonuniform grid at node $x = 0.5$.

k	10	50	100	200	500
Uniform grid	$(10, 10)$	$(50, 50)$	$(100, 100)$	$(200, 200)$	$(500, 500)$
Standard Modified	$8.3 * 10^{-2}$ $1.2 * 10^{-15}$	$5.0 * 10^{-1}$ $1.2 * 10^{-14}$	$9.9 * 10^{-1}$ $1.9 * 10^{-14}$	1.7355 $3.3 * 10^{-14}$	1.9988 $7.3 * 10^{-14}$
Nonuniform grid	$(5, 15)$	$(25, 75)$	$(50, 150)$	$(100, 300)$	$(250, 750)$
Standard Modified	5.0716 $2.6 * 10^{-15}$	2.6557 $1.4 * 10^{-14}$	2.9898 $3.0 * 10^{-14}$	2.3335 $4.0 * 10^{-14}$	2.3277 $1.6 * 10^{-13}$
Nonuniform grid	$(15, 5)$	$(75, 25)$	$(150, 50)$	$(300, 100)$	$(750, 250)$
Standard Modified	4.9774 $2.2 * 10^{-15}$	2.7337 $1.4 * 10^{-14}$	2.9816 $1.8 * 10^{-14}$	2.3740 $3.4 * 10^{-14}$	2.3366 $1.0 * 10^{-13}$

5. Numerical examples

To present the superiority of the modified schemes constructed both for uniform 3.5 and nonuniform 3.4 girds, we solve 2.1 on $\Omega = (0, 1) \subset \mathbb{R}$ for (a) when the Dirichlet boundary condition is applied at both ends given by

$$u(0) = 1 \quad \text{and} \quad u(1) = e^{ik} \tag{5.1}$$

and; (b) when the Dirichlet boundary condition is applied at the left end and the radiation boundary condition is applied at the right end given by

$$u(0) = 1 \quad \text{and} \quad u'(1) = iku(1). \tag{5.2}$$

Table 2. Comparison of dispersion errors for standard and modified central finite difference schemes for fixed $kh = 0.5$ with varying wave number for the case of boundary conditions 5.2 for a uniform grid and a three-point nonuniform grid at node $x = 0.5$.

k	10	50	100	200	500
Uniform grid	$(10, 10)$	$(50, 50)$	$(100, 100)$	$(200, 200)$	$(500, 500)$
Standard Modified	0.1151 $1.3 * 10^{-15}$	0.5292 $1.3 * 10^{-14}$	1.0292 $1.7 * 10^{-14}$	1.7550 $3.7 * 10^{-14}$	1.9957 $1.3 * 10^{-13}$
Nonuniform grid	$(5, 15)$	$(25, 75)$	$(50, 150)$	$(100, 300)$	$(250, 750)$
Standard Modified	1.5166 $1.8 * 10^{-15}$	2.0704 $1.2 * 10^{-14}$	1.8890 $2.6 * 10^{-14}$	2.0944 $4.8 * 10^{-14}$	2.1052 $1.2 * 10^{-13}$
Nonuniform grid	$(15, 5)$	$(75, 25)$	$(150, 50)$	$(300, 100)$	$(750, 250)$
Standard Modified	1.5166 $2.3 * 10^{-15}$	2.0704 $8.8 * 10^{-15}$	1.8890 $2.1 * 10^{-14}$	2.0944 $4.1 * 10^{-14}$	2.1052 $1.4 * 10^{-13}$

Table 3. Comparison of dispersion errors for standard and modified CFD schemes for fixed $h = 10^{-2}$ with varying wave number for the case of boundary conditions 5.1 (upper table) and 5.2 (lower table) for both (a) a uniform grid with 100 elements and (b) a three-point nonuniform grid at node $x = 0.5$ with $n_1 = 20$ and $n_2 = 80$ elements.

	(a) Uniform grid		(b) Nonuniform grid	
kh	Standard CFD scheme	Modified CFD scheme	Standard CFD scheme	Modified CFD scheme
10^{-2}	$1.1 * 10^{-6}$	$5.1 * 10^{-14}$	$1.7 * 10^{-1}$	$5.9 * 10^{-14}$
1	2.8621	$1.1 * 10^{-14}$	5.3181	$1.2 * 10^{-14}$
10	$9.9 * 10^{-1}$	$1.1 * 10^{-13}$	$9.9 * 10^{-1}$	$9.4 * 10^{-14}$
10^5	$9.9 * 10^{-1}$	$8.4 * 10^{-10}$	$9.9 * 10^{-1}$	$1.8 * 10^{-10}$
10^{12}	$9.9 * 10^{-1}$	$7.8 * 10^{-3}$	$9.9 * 10^{-1}$	$7.8 * 10^{-3}$

	(a) Uniform grid		(b) Nonuniform grid	
kh	Standard CFD scheme	Modified CFD scheme	Standard CFD scheme	Modified CFD scheme
10^{-2}	$1.3 * 10^{-5}$	$3.6 * 10^{-14}$	$3.0 * 10^{-1}$	$1.8 * 10^{-13}$
1	1.9999	$1.0 * 10^{-14}$	4.0474	$1.1 * 10^{-14}$
10	$9.9 * 10^{-1}$	$1.1 * 10^{-13}$	1.0059	$4.9 * 10^{-14}$
10^5	$9.9 * 10^{-1}$	$8.4 * 10^{-10}$	$9.9 * 10^{-1}$	$4.6 * 10^{-10}$
10^{12}	$9.9 * 10^{-1}$	$7.8 * 10^{-3}$	$9.9 * 10^{-1}$	$7.8 * 10^{-3}$

Moreover, the numerical error is measured using the discrete ℓ_∞ norm, defined by $\ell_\infty = \max_j |u_j - u(x_j)|, j = 0, 1, 2, \ldots, N$ with $u(x_j)$ representing the analytical solution and u_j the computed numerical solution. Moreover, N denotes the number of grid points in a uniformly spaced grid.

In Tables 1 and 2, dispersion errors with fixed $kh = 0.5$ for moderate range of wave numbers from $k = 10$ to $k = 500$ are given for both types of boundary conditions 5.1 and 5.2. It is evident that in the case of the standard CFD scheme for a uniform grid 2.5 dispersion error is less when $kh \ll 0$ compared with the standard CFD scheme for a nonuniform grid 2.4. Moreover, the dispersion error gets worse rapidly for increasing wave numbers even with fixed $kh = 0.5$, meaning that the dispersion error depends upon the nondimensional wave number kh. In the case of modified CFD schemes 3.4 and 3.5, it is evident from the dispersion error that highly accurate approximations of the numerical solutions are obtained irrespective of lower $k = 10$ and higher $k = 500$ wave numbers. Moreover, dispersion errors are given for two different mesh sizes around a three-point nonuniform grid at node $x = 0.5$ and the same behavior is observed for all schemes. Concluding accuracy of modified schemes is not deteriorated by choosing different numbers of elements around the node $x = 0.5$, which is not reflected in the case of standard CFD schemes.

Table 4. Comparison of dispersion error for standard and modified finite difference schemes for fixed $h = 10^{-2}$ with varying wave numbers for the case of boundary conditions 5.1 (upper table) and 5.2 (lower table) with (a) a uniform grid with 100 elements and (b) a three-point nonuniform grid at nodes $x = 0.1$ and $x = 0.7$ with $n_1 = 5$, $n_2 = 90$, and $n_3 = 5$ elements.

	(a) Uniform grid		(b) Nonuniform grid	
kh	Standard CFD scheme	Modified CFD scheme	Standard CFD scheme	Modified CFD scheme
10^{-2}	$1.6 * 10^{-4}$	$1.8 * 10^{-13}$	$7.7 * 10^{-4}$	$1.2 * 10^{-13}$
1	1.3555	$1.2 * 10^{-14}$	$9.9 * 10^{-1}$	$4.5 * 10^{-14}$
10	$9.9 * 10^{-1}$	$1.0 * 10^{-13}$	$9.9 * 10^{-1}$	$1.1 * 10^{-14}$
10^5	$9.9 * 10^{-1}$	$9.8 * 10^{-10}$	$9.9 * 10^{-1}$	$1.0 * 10^{-9}$
10^{12}	$9.9 * 10^{-1}$	$9.4 * 10^{-3}$	$9.9 * 10^{-1}$	$9.4 * 10^{-3}$

	(a) Uniform grid		(b) Nonuniform grid	
kh	Standard CFD scheme	Modified CFD scheme	Standard CFD scheme	Modified CFD scheme
10^{-2}	$2.1 * 10^{-5}$	$1.5 * 10^{-13}$	$4.1 * 10^{-4}$	$1.1 * 10^{-13}$
1	$1.0 * 10^{-14}$	$1.1 * 10^{-14}$	$1.3 * 10^{2}$	$1.1 * 10^{-14}$
10	$4.8 * 10^{-14}$	$1.3 * 10^{-13}$	$9.9 * 10^{-1}$	$1.3 * 10^{-13}$
10^5	$7.9 * 10^{-9}$	$8.6 * 10^{-9}$	$9.9 * 10^{-1}$	$9.4 * 10^{-9}$
10^{12}	$9.9 * 10^{-1}$	$9.3 * 10^{-3}$	$9.9 * 10^{-1}$	$1.0 * 10^{-2}$

In Tables 3 and 4, we present dispersion errors for kh ranging from 10^{-2} to 10^{12} for both types of boundary conditions 5.1 and 5.2. Moreover, in Table 3 dispersion results are presented for a single three-point nonuniform grid at the node $x = 0.5$, whereas in Table 4 dispersion results are presented for two three-point nonuniform grids at the nodes $x = 0.5$ and $x = 0.9$. Dispersion error is less for the standard CFD scheme for a uniform grid 2.5 compared with the standard CFD scheme for a three-point nonuniform grid 2.4, which is consistent with theory. However, this is the case only when kh is very small; with increasing kh even when $kh = 1$, the dispersion error gets worse for standard CFD schemes for both uniform and nonuniform grids. For the case of modified CFD schemes for both uniform and nonuniform grids, the dispersion error stays less for even extremely high $kh = 10^{12}$.

We also present a graphical comparison of standard and modified CFD schemes for a single and two three-point nonuniform grids considered at different nodes with different given wave numbers in Figures 1-4 and 5-6 respectively. Moreover, numerical approximations obtained with both standard and modified CFD schemes are shown for boundary conditions 5.1 and 5.2 in Figures 1–4 and 5–6, respectively. It is evident from Figures 1–4 that choosing a three-point node anywhere in the domain $(0, 1)$ for any fixed wave number k and any number

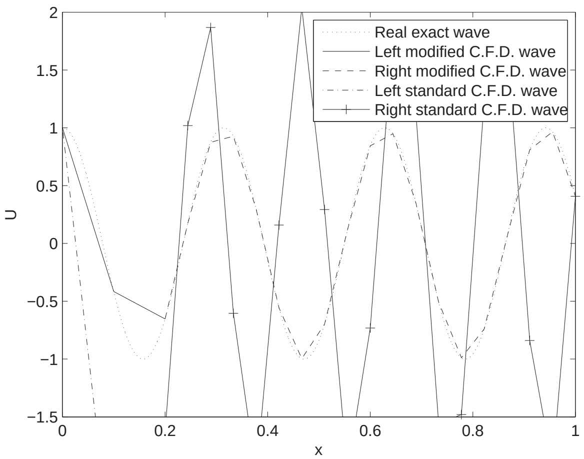

Figure 1. Comparison of dispersion errors for both standard and modified CFD schemes for boundary conditions 5.1 for a three-point nonuniform grid at $x = 0.2$ with $n_1 = 2$ and $n_2 = 18$ elements and $k = 20$.

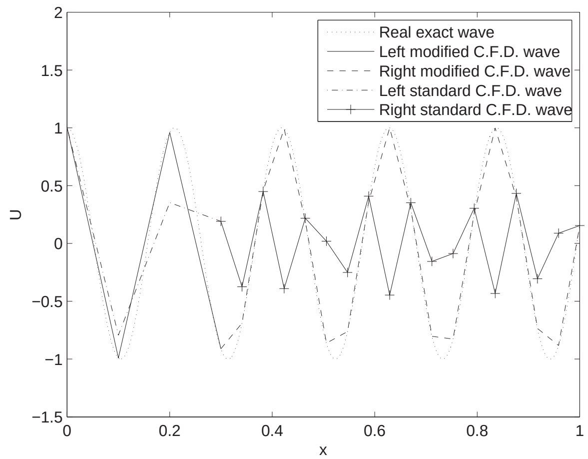

Figure 2. Comparison of dispersion errors for both standard and modified CFD schemes for boundary conditions 5.1 for a three-point nonuniform grid at $x = 0.3$ with $n_1 = 3$ and $n_2 = 17$ elements and $k = 30$.

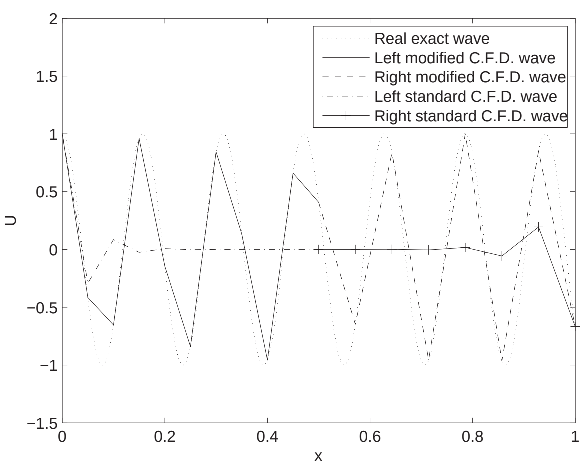

Figure 3. Comparison of dispersion errors for both standard and modified CFD schemes for boundary conditions 5.1 for a three-point nonuniform grid at $x = 0.5$ with $n_1 = 10$ and $n_2 = 7$ elements and $k = 40$.

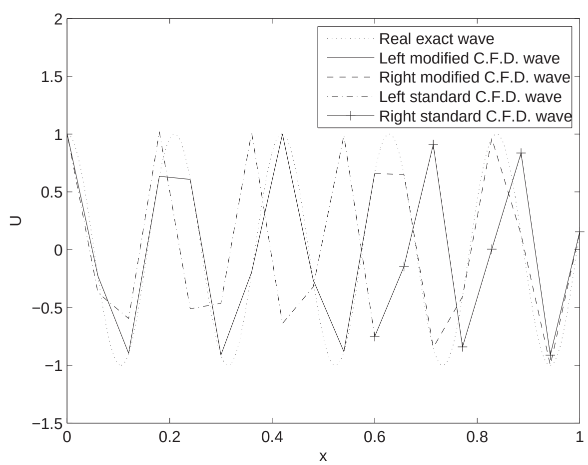

Figure 4. Comparison of dispersion errors for both standard and modified CFD schemes for boundary conditions 5.1 for a three-point nonuniform grid at $x = 0.6$ with $n_1 = 10$ and $n_2 = 7$ elements and $k = 30$.

of elements on either side of the node does not affect the accuracy of modified CFD approximations for the Helmholtz equation for boundary conditions 5.1. Nodally exact approximations are clearly showing that $k = \tilde{k}$ for the case of modified schemes. Meaning that both exact and numerical wave obtained using modified CFD scheme are oscillating with the same wave number, i.e. oscillation is both dispersion and dissipation-free. This is not the case for standard schemes where numerical approximations are affected by all position of grid nodes, number of elements on either side of the node, and the wave number. As overshoots Figure 1, undershoots Figure 2, nonoscillatory behavior Figure 3, and dispersive behavior Figure 4 is prominent. This behavior is

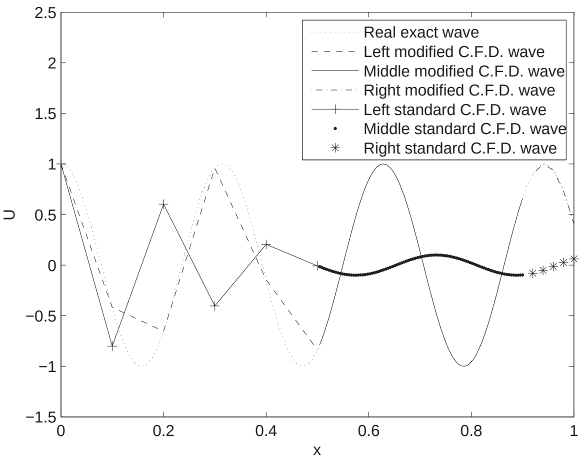

Figure 5. Comparison of dispersion errors for both standard and modified CFD schemes for boundary conditions 5.2 with $k = 20$ for two three-point nonuniform grids with $n_1 = 5, n_2 = 90$ and $n_3 = 5$ elements at $x = 0.5$ and $x = 0.9$.

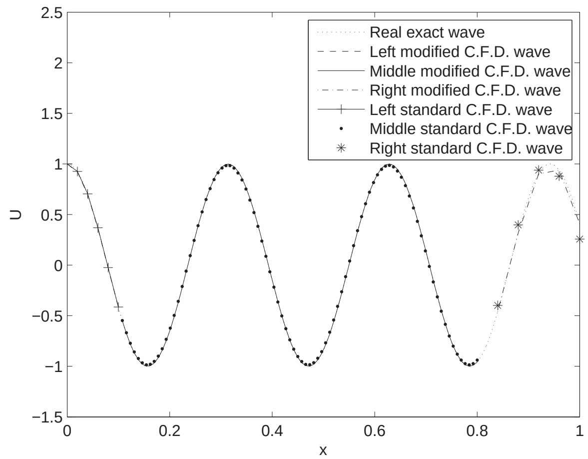

Figure 6. Comparison of dispersion errors for both standard and modified CFD schemes for boundary conditions 5.2 with $k = 20$ for two three-point nonuniform grids with $n_1 = 5, n_2 = 90$ and $n_3 = 5$ elements at $x = 0.1$ and $x = 0.8$.

heavily pronounced in the case of boundary conditions 5.2, where the radiation boundary condition is used at the right end (physically an outgoing wave). Placing grid nodes giving a three-point nonuniform grid does affect numerical approximations in the case of standard CFD schemes, which is clear from Figure 5 as the numerical wave obtained using standard schemes is not propagating where only changing nodes make it a traveling wave (Figure 6) for the same given wave number $k = 20$. In contrast, the numerical wave obtained using the modified CFD scheme is propagating without dispersion and dissipation.

6. Conclusions

A modified central finite difference scheme for a three-point nonuniform grid is constructed for the one-dimensional Helmholtz equation using the idea of *Bloch wave property* originally presented in [21] for uniform grids specifically presented for the simulations of waves traveling with large wave numbers (or equally good frequency). The modified CFD scheme for a nonuniform grid provides

1. highly accurate finite difference solutions at the nodes of the nonuniform grid for all range of wave numbers irrespective of how the grid is adapted throughout the domain;

2. adds no additional cost to the implementation and keeps the same stencil structure (tri-diagonal) one has in the case of standard schemes;

3. dispersion error is independent of both wave number k and the mesh size h and as a result provides highly accurate numerical solutions even for large wave numbers (equally good frequency), which is not in the scope of standard CFD schemes at all.

However, construction of modified central finite difference schemes for the nonhomogeneous Helmholtz equation and extension to higher dimensions is part of future work.

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