High-Order Non-Reflecting Boundary Conditions for Dispersive Waves

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Abstract

Problems of linear time-dependent dispersive waves in an unbounded domain are considered. The infinite domain is truncated via an artificial boundary $\mathcal{B}$, and a high-order Non-Reflecting Boundary Condition (NRBC) is imposed on $\mathcal{B}$. Then the problem is solved by a Finite Difference scheme in the finite domain bounded by $\mathcal{B}$. The sequence of NRBCs proposed by Higdon is used. However, in contrast to the original low-order implementation of the Higdon conditions, a new scheme is devised which allows the easy use of a Higdon-type NRBC of *any* desired order. In addition, a procedure for the automatic choice of the parameters appearing in the NRBC is proposed. The performance of the scheme is demonstrated via numerical examples.

Keywords: Waves, High-order, Artificial boundary, Non-reflecting boundary condition, Higdon, Finite Difference.

1. Introduction

In many fields of application involving the propagation of waves, the domain of the problem under investigation is unbounded (or very large). One of the common methods used for the numerical solution of such problems [1] is the method of Non-Reflecting Boundary Conditions. In this method the original domain is truncated via an artificial boundary $\mathcal{B}$, thus forming a finite computational domain Ω bounded by $\mathcal{B}$. A special boundary condition is imposed on $\mathcal{B}$, in order to complete the statement of the problem (i.e., make the solution unique) and, most importantly, to ensure that no (or little) spurious wave reflection occurs from $\mathcal{B}$. Then the problem is solved numerically in Ω.

The boundary condition applied on $\mathcal{B}$ is called a Non-Reflecting Boundary Condition (NRBC), although a few other names are often used too [2]. Naturally, the quality of the numerical solution strongly depends on the properties of the NRBC employed. In the last 25 years or so, much research has been done to develop NRBCs that after discretization lead to a scheme which is stable, accurate, efficient and easy to implement. See [3] and [4] for recent reviews on the subject. Of course, it is difficult to find a single NRBC which is ideal in all respects and all cases; this is why the quest for better NRBCs and their associated discretization schemes continues.

Some low-order local NRBCs have been proposed in the late 70's and early 80's and have become well-known, e.g., the Engquist-Majda NRBCs [5] and the Bayliss-Turkel NRBCs [6]. The late 80's and early 90's have been characterized by the emerging of the exact nonlocal Dirichlet-to-Neumann (DtN) NRBC [7, 8] and the Perfectly Matched Layer (PML) [9]. More recently, *high-order* local NRBCs have been introduced. Sequences of increasing-order NRBCs have been available before (e.g., the Bayliss-Turkel conditions [6] constitute such a sequence), but they had been regarded as impractical beyond 2nd or 3rd order from the implementation point of view. Only since the mid 90's, practical high-order NRBCs have been devised.

The first such high-order NRBC has apparently been proposed by Collino [10], for two-dimensional time-dependent waves in rectangular domains. Its construction requires the solution of the one-dimensional wave equation on $\mathcal{B}$. Grote and Keller [11] developed a high-order converging NRBC for the three-dimensional time-dependent wave equation, based on spherical harmonic transformations. They extended this NRBC for the case of elastic waves in [12]. Sofronov [13] has independently published a similar scheme in the Russian literature. Hagstrom and Hariharan [14] constructed high-order NRBCs for the two- and three-dimensional time-dependent wave equations based on the analytic series representation for the outgoing solutions of these equations. It looks simpler than the previous two NRBCs. For time-dependent waves in a two-dimensional wave guide, Guddati and Tassoulas [15] devised a high-order NRBC by using rational approximations and recursive continued fractions. Givoli [16] has shown how to derive high-order NRBCs for a general class of wave problems, leading to a symmetric finite element formulation. In [17], this methodology was applied to the particular case of time-harmonic waves, using optimally localized DtN NRBCs.

Most of the NRBCs mentioned above have been designed for either time-harmonic waves

or for non-dispersive time-dependent waves. The presence of *wave dispersion* makes the time-dependent problem much more difficult as far as NRBC treatment is concerned. Dispersive media appear in various applications. One important example is that of meteorological models which take into account the earth rotation [18]. Other examples include quantum-mechanics waves, the vibration of structures with rotational rigidity such as beams, plates and shells, and many nonlinear wave problems, with or without linearization. Very recently, Navon et al. [19] developed a PML scheme for the dispersive shallow water equations. In the present paper we develop high-order NRBCs for dispersive waves. Naturally, our scheme is just as applicable to the non-dispersive case, by simply taking the dispersion parameter to be zero.

Higdon [20] proposed a sequence of NRBCs for the dispersive (Klein-Gordon) wave equation. In fact, these NRBCs were developed originally for non-dispersive waves [21]–[25], but Higdon showed in [20] that they can be applied in the dispersive case too. Indeed, our scheme is based on Higdon's NRBCs. However, in contrast to the original low-order formulation of these conditions, a new scheme is devised here which allows the easy use of a Higdon-type NRBC of *any* desired order. In addition, a procedure for the automatic choice of the parameters appearing in the NRBC is proposed.

Following is the outline of the rest of this paper. In Section 2 we state the problem under investigation. We emphasize that the setup taken here, namely that of a semi-infinite wave guide, serves merely as an example, and in fact the proposed approach is general and can easily be extended to other configurations, such as two-dimensional exterior problems with a rectangular artificial boundary. In Section 3 we present the Higdon NRBCs and briefly recall their properties. In Section 4 we show how to implement the Higdon NRBCs, using a Finite Difference (FD) scheme, in a high-order way. Then we show, in Section 5, how the basic FD approximations used in this scheme can be improved if one desires, and in Section 6 we present a procedure for the automatic choice of the NRBC parameters. We demonstrate the performance of the new method via some numerical examples in Section 7. We conclude, in Section 8, with some remarks.

2. Statement of the Problem

We consider the linear inhomogeneous Klein-Gordon equation,

$$\partial_t^2 u - C_0^2 \nabla^2 u + f^2 u = S \ , \tag{1}$$

in a two-dimensional uniform semi-infinite channel or wave guide. A Cartesian coordinate system (x, y) is introduced such that the wave-guide is parallel to the x direction. The width of the wave-guide is denoted b. The setup is shown in Fig. 1(a). In (1), u is the unknown wave field, C_0 is the given reference wave speed, f is the given dispersion parameter, and S is a given wave source function. The C_0 and f are allowed to be functions of location; however, it is assumed that the region where they are not constant is finite (and typically located near the west boundary Γ_W). The wave source S is a function of location and time, but it

is assumed to have a local support. Eq. (1) describes, for example, the lateral vibration of a membrane strip on an elastic foundation, or the acoustic pressure in a dispersive medium (say, a linearized bubbly medium). Also, it can be shown that the linearized shallow water equations, with a flat bottom and zero initial conditions, reduce to (1), where u is the water elevation above the reference level [18]. In the geophysical context, f is called the Coriolis parameter and is related to the angular velocity of the earth.

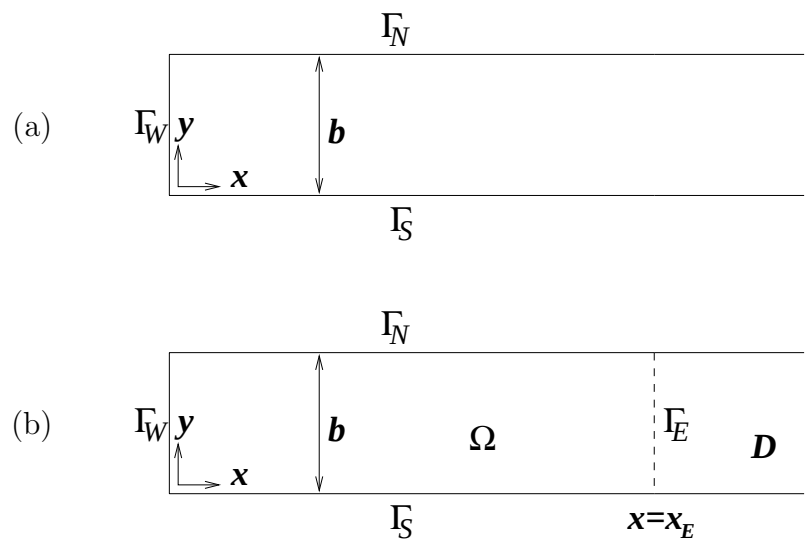

Figure 1: Setup for the wave-guide problem: (a) the original problem in a semi-infinite wave guide; (b) the computational problem in a finite domain Ω.

On the south and north boundaries Γ_S and Γ_N we specify the Neumann condition:

$$\partial_y u = 0 \qquad \text{on} \quad \Gamma_S \quad \& \quad \Gamma_N \ . \tag{2}$$

In acoustics this corresponds to a "hard wall" condition. On the west boundary Γ_W we prescribe u using a Dirichlet condition, i.e.,

$$u(0, y, t) = u_W(y, t) \qquad \text{on} \quad \Gamma_W \ , \tag{3}$$

where $u_W(y, t)$ is a given function (incoming wave). At $x \to \infty$ the solution is known to be bounded and not to include any incoming waves.

To complete the statement of the problem, the initial conditions

$$u(x, y, 0) = u_0 \qquad , \qquad \partial_t u(x, y, 0) = v_0 \ , \tag{4}$$

are given at time $t = 0$ in the entire domain. We assume that the functions u_0 and v_0 have a local support.

We now truncate the semi-infinite domain by introducing an artificial east boundary $\mathcal{B} \equiv \Gamma_E$, located at $x = x_E$. See Fig. 1(b). This boundary divides the original semi-infinite domain into two subdomains: an exterior domain D, and a finite computational domain Ω which is bounded by Γ_W, Γ_N, Γ_S and Γ_E. We choose the location of Γ_E such that the entire support of S, u_0 and v_0 and the region of non-uniformity of C_0 and f are all contained inside Ω. Thus, on Γ_E and in D, the homogeneous counterpart of (1) holds, i.e.,

$$\partial_t^2 u - C_0^2 \nabla^2 u + f^2 u = 0 \ , \tag{5}$$

with constant coefficients C_0 and f^2, and the medium is initially at rest.

To obtain a well-posed problem in the finite domain Ω we need to impose a boundary condition on Γ_E. This must be a Non-Reflecting Boundary Condition (NRBC), so as to prevent spurious reflection of waves. In the next section we discuss the choice of this NRBC.

3. Higdon's NRBCs

On the artificial boundary Γ_E we use one of the *Higdon NRBCs* [20]. These NRBCs were presented and analyzed in a sequence of papers [21]–[25] for non-dispersive acoustic and elastic waves, and were extended in [20] for the dispersive case. The Higdon NRBC of order J is

$$H_J : \qquad \left[\prod_{j=1}^{J} \left(\partial_t + C_j \partial_x \right) \right] u = 0 \qquad \text{on} \quad \Gamma_E \ . \tag{6}$$

Here, the C_j are parameters which have to be chosen and which signify phase speeds in the x-direction. The main advantages of the Higdon conditions are as follows:

- The Higdon NRBCs are very *general*, namely they apply to a variety of wave problems, in one, two and three dimensions and in various configurations. Moreover, they can be used, without any difficulty, for *dispersive* wave problems and for problems with layers. Most other available NRBCs are either designed for non-dispersive homogeneous media (as in acoustics and electromagnetics) or are inherently of low order (as in meteorology and oceanography).

- The Higdon NRBCs constitute a *sequence* of conditions of increasing order. This, and the fact that no asymptotic approximation is involved in their construction, enables one in principle (leaving implementational issues aside for the moment) to obtain solutions with unlimited accuracy.

- For certain choices of the parameters, the Higdon NRBCs are equivalent to NRBCs that are derived from rational approximation of the dispersion relation (the Engquist-Majda conditions [5] being the most well-known example). This has been proved by Higdon in [20, 21]. More precisely, Higdon's theorem states that if a NRBC is based on a symmetric rational approximation to the dispersion relation corresponding to

outgoing waves, then it is either (a) equivalent to (6) for a suitable choice of J and the parameters C_j, or (b) unstable, or (c) not optimal. Lack of optimality means here that the coefficients in the NRBC can be modified so as to reduce the amount of the spurious reflection. Thus, the Higdon NRBCs can be viewed as generalization of rational-approximation NRBCs.

The scheme developed here is different than the original Higdon scheme [20] in the following ways:

(a) The discrete Higdon conditions were developed in the literature up to third order only, because of their algebraic complexity which increases rapidly with the order. Here we show how to easily implement these conditions to an *arbitrarily high order*. The scheme is coded once and for all for any order; the order of the scheme is simply an input parameter.

(b) The Higdon NRBCs involve some parameters which must be chosen. Higdon [20] discusses some general guidelines for their manual a-priori choice by the user. We shall show how these parameters can be chosen *automatically*.

(c) We shall show how to improve the discretization of the basic operators involved in the Higdon NRBCs, by using more accurate FD stencils, and how to incorporate these improved discretizations in the new scheme.

We now make a few remarks recalling the properties of the Higdon NRBCs.

1. The boundary condition (6) is exact for all waves that propagate with an x-direction phase speed equal to either of $C_1, \ldots, C_J$. To see this, consider a wave which satisfies the wave equation (5) with constant C_0 and f. Such a wave has the form

$$u = A \cos \frac{n\pi y}{b} \cos(kx - \omega t + \psi) \ , \tag{7}$$

where

$$\omega^2 = C_0^2 \left(k^2 + \frac{n^2 \pi^2}{b^2} \right) + f^2 \qquad , \qquad n = 0, 1, 2, \ldots \tag{8}$$

Also, let

$$C_x = \frac{\omega}{k} \ , \tag{9}$$

which is the x-direction phase velocity. In (7)–(9), A is the wave amplitude, ψ is its phase, k is the x-component wave number, and ω is the wave frequency. Eq. (8) is the dispersion relation. In general, solutions of (5) consist of an infinite number of waves of the form (7). There are also solutions that decay exponentially in the x direction; however, they are usually not of great concern, since the decaying modes are expected to be insignificant at the time they reach Γ_E. Now, it is easy to verify that if one of the C_j's in (6) is equal to C_x, then the wave (7) satisfies the boundary condition (6) exactly.

2. From (8) and (9) we have

$$C_x = \sqrt{C_0^2 + \frac{C_0^2 n^2 \pi^2 / b^2 + f^2}{k^2}} \qquad , \qquad n = 0, 1, 2, \ldots \tag{10}$$

   Thus, always $C_x \geq C_0$; hence one should take $C_j \geq C_0$.

3. The first-order condition H_1 is a Sommerfeld-like boundary condition. If we set $C_1 = C_0$ we get the classical Sommerfeld-like NRBC. A lot of work in the meteorological literature is based on using H_1 with a specially chosen C_1. Pearson [26] used a special but constant value of C_1, while in the scheme devised by Orlanski [27] and in later improved schemes [28]–[31] the C_1 changes dynamically and locally in each time-step based on the solution from the previous time-step. Some of the limited-area weather prediction codes used today are based on such schemes, e.g., COAMPS [32]. See also the recent papers [33]–[35] where several such adaptive H_1 schemes are compared.

4. The condition H_J involves normal and temporal derivatives up to Jth-order. In fact, it has the form

$$\sum_{j=0}^{J} w_j \; \partial_x^j \partial_t^{J-j} u = 0 \; , \tag{11}$$

   which is obtained by expanding (6). Finding the general formula for the coefficients w_j in (11) is difficult, but fortunately we shall not need it in our new scheme.

5. It is easy to show (see Higdon [20] for a similar setting) that when a wave of the form (7) impinges on the boundary Γ_E where the NRBC H_J is imposed, the resulting *reflection coefficient* is

$$R = \prod_{j=1}^{J} \left| \frac{C_j - C_x}{C_j + C_x} \right| \; . \tag{12}$$

   Again we see that if $C_j = C_x$ for any one of the j's then $R = 0$, namely there is no reflection and the NRBC is exact. Moreover, we see that the reflection coefficient is a product of J factors, *each of which is smaller than 1.* This implies that the reflection coefficient becomes smaller as the order J increases regardless of the choice made for the parameters C_j. Of course, a good choice for the C_j would lead to better accuracy with a lower order J, but even if we miss the correct C_j's considerably (say, if we make the simplest choice $C_j = C_0$ for $j = 1, \ldots, J$), we are still guaranteed to reduce the spurious reflection as we increase the order J. This is an important property of the Higdon's NRBCs and is the reason for their robustness.

6. In [23], Higdon points to the possibility of a long-time instability that might occur when one uses a NRBC with high-order derivatives. If the interior governing equations and the NRBC both admit solutions at zero wave number and frequency, and if the data in the problem include such "zero modes," then a slowly-growing smooth instability is possible. Whether this shows up in practice depends on the order of the derivatives

in the NRBC and on the number of spatial dimensions. However, these difficulties do not arise in the presence of dispersion, or if the data are confined to nontrivial modes.

4. Discretization of Higdon's NRBCs

The Higdon condition H_J given by (6) is a product of J operators of the form $\partial_t + C_j \partial_x$. Consider the following FD approximations:

$$\partial_t \simeq \frac{I - S_t^-}{\Delta t} \qquad , \qquad \partial_x \simeq \frac{I - S_x^-}{\Delta x} \ . \tag{13}$$

In (13), Δt and Δx are, respectively, the time-step size and grid spacing in the x direction, I is the identity operator, and S_t^- and S_x^- are shift operators defined by

$$S_t^- u_{pq}^n = u_{pq}^{n-1} \qquad , \qquad S_x^- u_{pq}^n = u_{p-1,q}^n \ . \tag{14}$$

Here and elsewhere, u_{pq}^n (and also $u_{p,q}^n$) is the FD approximation of $u(x, y, t)$ at grid point (x_p, y_q) and at time t_n. We use (13) in (6) to obtain:

$$\left[\prod_{j=1}^{J} \left(\frac{I - S_t^-}{\Delta t} + C_j \frac{I - S_x^-}{\Delta x} \right) \right] u_{Eq}^n = 0 \ . \tag{15}$$

Here, the index E correspond to a grid point on the boundary Γ_E. Higdon has solved this difference equation (and also a slightly more involved equation that is based on time- and space-averaging approximations for ∂_x and ∂_t; see next section) for $J \leq 3$ to obtain an explicit formula for u_{Eq}^n. This formula is used to find the current values on the boundary Γ_E *after* the solution in the interior points and on the other boundaries has been updated; thus it is an explicit formula. The formula for $J = 2$ is found in [25], and the one for $J = 3$ appears in the appendix of [24]. The algebraic complexity of these formulas increases rapidly with the order J. It is thus not surprising that we have not found in the literature any report on the implementation of the Higdon NRBCs beyond $J = 3$.

Now we show how to implement the Higdon NRBCs *to any order* using a simple algorithm. To this end, we first multiply (15) by Δt and rearrange to obtain

$$Z \equiv \left[\prod_{j=1}^{J} \left(a_j I + d_j S_t^- + e_j S_x^- \right) \right] u_{Eq}^n = 0 \ , \tag{16}$$

where

$$a_j = 1 + \frac{C_j \Delta t}{\Delta x} \ , \tag{17}$$

$$d_j = -1 \ , \tag{18}$$

$$e_j = -\frac{C_j \Delta t}{\Delta x} \ . \tag{19}$$

The coefficient d_j actually does not depend on j, but we keep this notation to allow easy extensions to the scheme (see next section). Now, Z in (16) can be written as a sum of 3^J terms, each one is an operator acting on u^n_{Eq}, namely

$$Z \equiv \sum_{m=0}^{3^J-1} A_m P_m u^n_{Eq} = 0 \ . \tag{20}$$

Here A_m is a coefficient depending on the a_j, d_j and e_j, and P_m is an operator involving products of I, S_t^- and S_x^-. All the terms in the sum in (20) are computable at the current time step n, except the one which involves only the identity operator and no shift operators. If we let this term correspond to $m = 0$, then $P_0 = I$ and

$$A_0 = \prod_{j=1}^{J} a_j \ . \tag{21}$$

Thus we get from (20)

$$Z \equiv A_0 u^n_{Eq} + Z^* = 0 \ , \tag{22}$$

where

$$Z^* = \sum_{m=1}^{3^J-1} A_m P_m u^n_{Eq} \ . \tag{23}$$

From (22) we get

$$u^n_{Eq} = -Z^*/A_0 \ , \tag{24}$$

which is the desired value of u on the boundary Γ_E.

The problem now reduces to calculating Z^* given by (23). We do this using the algorithm described in Box 1. The basic idea is to calculate the coefficients A_m and the operator actions $P_m u^n_{Eq}$ term by term. This is done systematically by transforming the integer counter m to a number in base 3 with J digits. The A_m and P_m are not simple functions of the decimal representation of the number m, but they *are* simple functions of the digits of the base-3 representation of m.

Note that we need to store $u^{\hat{n}}_{\hat{i}q}$ values for $\hat{i} = E, E-1, \ldots, E-J$ and $\hat{n} = n, n-1, \ldots, n-J$. In other words, we have to store the history of the values of u for a layer of thickness $J+1$ points near the boundary Γ_E and for $J+1$ time levels (including the current one). If there are N_y grid points in the y direction, then the amount of storage needed in a simple storage scheme is $(J+1)^2 N_y$. However, one can save in storage by exploiting the fact that not all values $u^{\hat{n}}_{\hat{i}q}$ are needed, but only those for which $(E-\hat{i}) + (n-\hat{n}) \leq J$. This is clear from (11) and also from (16). For example, the solution at time t_{n-J} should be stored only for points on the boundary Γ_E itself.

Higdon [20] has proved, in the context of the scalar Klein-Gordon equation (5), that the discrete NRBCs (15) are stable if the interior scheme is the standard *second-order centered*

- Start with $Z^* = 0$. Calculate $A_0 = \prod_{j=1}^{J} a_j$.
- Loop over the integers $m = 1, \ldots, 3^J - 1$.
  - For a given m, transform m into a number r in base 3, consisting of the digits 0, 1 and 2 only. The length of r will be at most J digits. Store the J digits of r in the vector $D_r(j)$, $j = 1, \ldots, J$.
    Example: Suppose that $J = 6$ and $m = 227$. Since 227 in base 3 is $r = 22102$, we will get $D_r = \{\ 0\ 2\ 2\ 1\ 0\ 2\ \}$.
  - Use D_r to calculate the coefficient A_m. To this end, start with $A_m = 1$, loop over $j = 1, \ldots, J$, and for each j multiply A_m by the factor a_j (if $D_r(j) = 0$) or d_j (if $D_r(j) = 1$) or e_j (if $D_r(j) = 2$).
    Example: For $J = 6$ and $m = 227$, we have received the vector D_r above. Then $A_{227} = a_1 e_2 e_3 d_4 a_5 e_6$.
  - Use D_r to calculate the operator action $P_m u^n_{Eq}$. To this end, start with $\hat{n} = n$ and $\hat{i} = E$, loop over $j = 1, \ldots, J$, and for each j subtract 1 from $\hat{n}$ (if $D_r(j) = 1$) or subtract 1 from $\hat{i}$ (if $D_r(j) = 2$) or do nothing (if $D_r(j) = 0$). After the loop ends we have $P_m u^n_{Eq} = u^{\hat{n}}_{\hat{i}q}$.
    Example: For the case $J = 6$ and $m = 227$ considered above, we get $\hat{n} = n - 1$ (because the digit "1" appears only once in D_r), and $\hat{i} = E - 3$ (because the digit "2" appears three times in D_r). Hence $P_{227} u^n_{Eq} = u^{n-1}_{E-3,q}$.
  - Update: $Z^* \leftarrow Z^* + A_m u^{\hat{n}}_{\hat{i}q}$.
- Next m.
- $u^n_{Eq} = -Z^*/A_0$.

Box 1. Algorithm for implementing the Higdon NRBC of order J.

difference scheme

$$u_{pq}^{n+1} = 2u_{pq}^{n} - u_{pq}^{n-1} + \left(\frac{C_0\Delta t}{\Delta x}\right)^2 \left(u_{p+1,q}^{n} - 2u_{pq}^{n} + u_{p-1,q}^{n}\right) + \left(\frac{C_0\Delta t}{\Delta y}\right)^2 \left(u_{p,q+1}^{n} - 2u_{pq}^{n} + u_{p,q-1}^{n}\right) - (f\Delta t)^2 u_{pq}^{n} \ . \tag{25}$$

We use this interior scheme in the numerical experiments presented in Section 7. Since both (25) and the discretized Higdon NRBC are explicit, the whole scheme is explicit.

An alternative formulation of the Higdon NRBC, where all the high-order derivatives are eliminated by the use of auxiliary variables, is currently under development and will be reported in a future publication.

5. Improved Discrete Higdon NRBCs

The discretization scheme described in the previous section is based on the basic FD approximations given by (13). These approximations can be improved in several ways. For example:

(a) We can take

$$\partial_t \simeq \frac{I - S_t^-}{\Delta t}\left((1-b)I + bS_x^-\right) \quad , \quad \partial_x \simeq \frac{I - S_x^-}{\Delta x}\left((1-b)I + bS_t^-\right) \ , \tag{26}$$

where $0 \le b \le 1$. Thus, the temporal difference is calculated with a weighted average in space while the spatial difference is calculated with a weighted averaged in time. The formulas (13) correspond to $b = 0$. In [20], Higdon has used this approximation with $b = 0.5$, and reported a slight improvement in the results compared to the use of (13).

(b) We can take one-sided approximations for the x- and t-derivatives [36], i.e.,

$$\partial_t \simeq \frac{3I - 4S_t^- + (S_t^-)^2}{2\Delta t} \quad , \quad \partial_x \simeq \frac{3I - 4S_x^- + (S_x^-)^2}{2\Delta x} \ . \tag{27}$$

These approximations are second-order accurate, as opposed to those in (13) which are first-order accurate.

(c) We can combine the two types of approximations given above, namely

$$\partial_t \simeq \frac{3I - 4S_t^- + (S_t^-)^2}{2\Delta t}\left((1-b)I + bS_x^-\right) \ , \quad \partial_x \simeq \frac{3I - 4S_x^- + (S_x^-)^2}{2\Delta x}\left((1-b)I + bS_t^-\right) \ . \tag{28}$$

The procedure described in the previous section for implementing the Higdon NRBCs can easily be modified to admit each of these improved approximations. The main feature that has to be changed in the algorithm outlined in Box 1 is the *base* to which the counting decimal integer m is transformed. For example, consider the weighted approximation (26) replacing (13). In this case (16), which involves three basic operators (I, S_t^- and S_x^-) is replaced by

$$Z \equiv \left[\prod_{j=1}^{J} \left(a_j I + d_j S_t^- + e_j S_x^- + g_j S_t^- S_x^- \right) \right] u_{Eq}^n = 0 \ , \tag{29}$$

which involves *four* basic operators (I, S_t^-, S_x^- and $S_t^- S_x^-$). Therefore, the counter m in the main loop in Box 1 will range from 1 to $4^J - 1$, and all the calculation will be performed in base 4 rather than in base 3. Similarly, the approximations (27) and (28) will require calculations in base 5 and base 8, respectively. The alternations needed in the coding are minor, but naturally the computational time associated with these improved approximations would increase dramatically.

We note that when one uses a high-order Higdon NRBC, the discrete operator involved is of high-order even when the simplest formulas (13) are used to approximate the x- and t-derivatives. Thus, the importance of the improvements discussed above diminishes when J increases. In fact, it is probably worthwhile to incorporate such improvements in the scheme only if a low-order condition (say, $J \leq 3$) is employed.

6. Controlling the Parameters

The Higdon NRBCs involve the parameters C_j which must be chosen. There are three approaches in this context:

(a) The user chooses the C_j a-priori in a manual manner based on an "educated guess." This is the procedure recommended in Higdon's papers [20]–[25].

(b) The C_j are chosen automatically by the computer code as a preprocess.

(c) The C_j are not constant, but are determined dynamically by the computer code. Namely, a value for C_j is estimated for every grid point on the boundary at each time step, from the solution in the previous time-steps.

We have adopted approach (b), which is automatic yet very inexpensive computationally. The algorithm we propose is described in Box 2. It is based on the *maximum resolvable* wave numbers in the x and y directions, and on the minimax formula [37] for choosing the x-component wave numbers.

- Given the grid parameter Δx, estimate the maximum resolvable wave number k in the x direction. Assuming a maximum of 10 grid points per wave length, a reasonable estimate is
$$k_{\max} = \frac{\pi}{5\Delta x} \ .$$
- Choose $J-1$ values of k from the interval $(0, k_{\max})$. This is done using the symmetric minimax formula (based on the Chebyshev polynomial) proposed by Sommeijer et al. [37]:
$$k_j = \left[\frac{k_{\max}^2}{2}\left(1+\cos\left(\frac{2j-1}{2(J-1)}\pi\right)\right)\right]^{\frac{1}{2}} \ , \qquad j = 1, \ldots, J-1 \ .$$
- Given the grid parameter Δy, estimate the maximum resolvable wave number k_y in the y direction. Again assuming a maximum of 10 grid points per wave length, a reasonable estimate is
$$(k_y)_{\max} = \frac{\pi}{5\Delta y} \ .$$
- For each k_j, calculate the corresponding (and maximal in the y direction) frequency ω_j from the dispersion relation (8):
$$\omega_j = \sqrt{C_0^2\left[k_j^2 + (k_y)_{\max}^2\right] + f^2} \ .$$
- Calculate
$$C_j = \frac{\omega_j}{k_j} \qquad \text{for} \quad j = 1, \ldots, J-1 \ .$$
- Add the value C_0 (the minimum possible phase speed) to the $J-1$ values calculated above. These constitute the desired J values C_j.

Box 2. Algorithm, used as a preprocess, for determining the parameters C_j in the Higdon NRBC.

7. Numerical examples

We first apply the new scheme to a simple test problem whose exact solution is synthesized a priori. We consider the wave-guide problem described in Section 2 and illustrated in Fig. 1(a). We set $b = 5$, $C_0 = 1$ and $f = 0.5$. The boundary function $u_W(y,t)$ on Γ_W and the initial conditions are those that correspond to a solution $u(x,y,t)$ which is a linear combination of three waves of the form (7), i.e.,

$$u = \sum_{m=1}^{3} A_m \cos\frac{n_m \pi y}{b} \cos(k_m x - \omega_m t) \ . \tag{30}$$

The parameters chosen in (30) are:
$A_m = 1, \quad 1, \quad 1 \ ;$
$n_m = 1, \quad 2, \quad 2 \ ;$
$\omega_m = 0.81, \quad 1.37, \quad 1.68 \ .$
This corresponds to the three phase velocities (obtained from (10)):
$C_x/C_0 = 7.61, \quad 6.27, \quad 1.69 \ .$
The k_m in (30) are obtained from the ω_m and the n_m via the dispersion relation (8).

We introduce the artificial boundary Γ_E (see Fig. 1(b)) at $x_E = 5$. Thus, the computational domain Ω is a 5×5 square. In Ω we use a uniform grid with 21×21 points. We discretize the Klein-Gordon equation in Ω using the explicit central-difference FD interior scheme (25). On Γ_E we impose the Higdon NRBC implemented in its high-order form. The time-step size is $\Delta t = 0.025$, which is smaller than the CFL limit and thus guarantees stability.

In Figs. 2(a)–(d), we plot the solution u at the point $x = 5$, $y = 2.75$ (located on Γ_E) as a function of time. In each of the four figures the exact solution is compared to a number of numerical solutions obtained with different NRBC schemes, namely with different choices of the order J and the parameters C_j. First we choose $C_j = 1$ for all j. Fig. 2(a) shows the H_1, H_2 and H_3 solutions. Their accuracy is poor, although the H_3 solution is significantly better than the other two. Fig. 2(b) shows the H_5 and H_7 solutions. The H_7 solution is quite accurate in the entire time interval shown. Thus, if the C_j's are not specially chosen, we need the order of the Higdon NRBC to be as high as 7 for high accuracy.

Now we employ the procedure given by Box 2 to automatically choose the C_j's. Fig. 2(c) shows the resulting H_3, H_4 and H_5 solutions. We see that in this case the approach of the numerical solutions to the exact solution is monotone. Moreover, for $J = 5$ we get about the same level of accuracy as we did with $J = 7$ when all the C_j had the value one (Fig. 2(b)). For additional reference, we show in Fig. 2(d) the H_3 solution obtained with the C_j corresponding to the three phase velocities C_x of the exact solution. It is about as accurate as the H_5 solution in Fig. 2(c). We also show the H_4 solution obtained with the exact C_1, C_2, C_3 and with $C_4 = 1$. The numerical solution is indistinguishable from the exact solution. In this case not only the NRBC is exact, but we gain additional accuracy on the boundary due to the increased order of the FD scheme.

This example demonstrates, albeit in a simplified setting, that the same level of accuracy

obtained with parameter values C_j that are well-estimated can be achieved with ill-chosen parameter values but with an increased order J. Of course, increasing the order to ensure high accuracy is computationally expensive, and therefore it is usually beneficial to use the algorithm given in Box 2.

We now consider another problem in the same wave-guide, again with $b = 5$, $C_0 = 1$ and

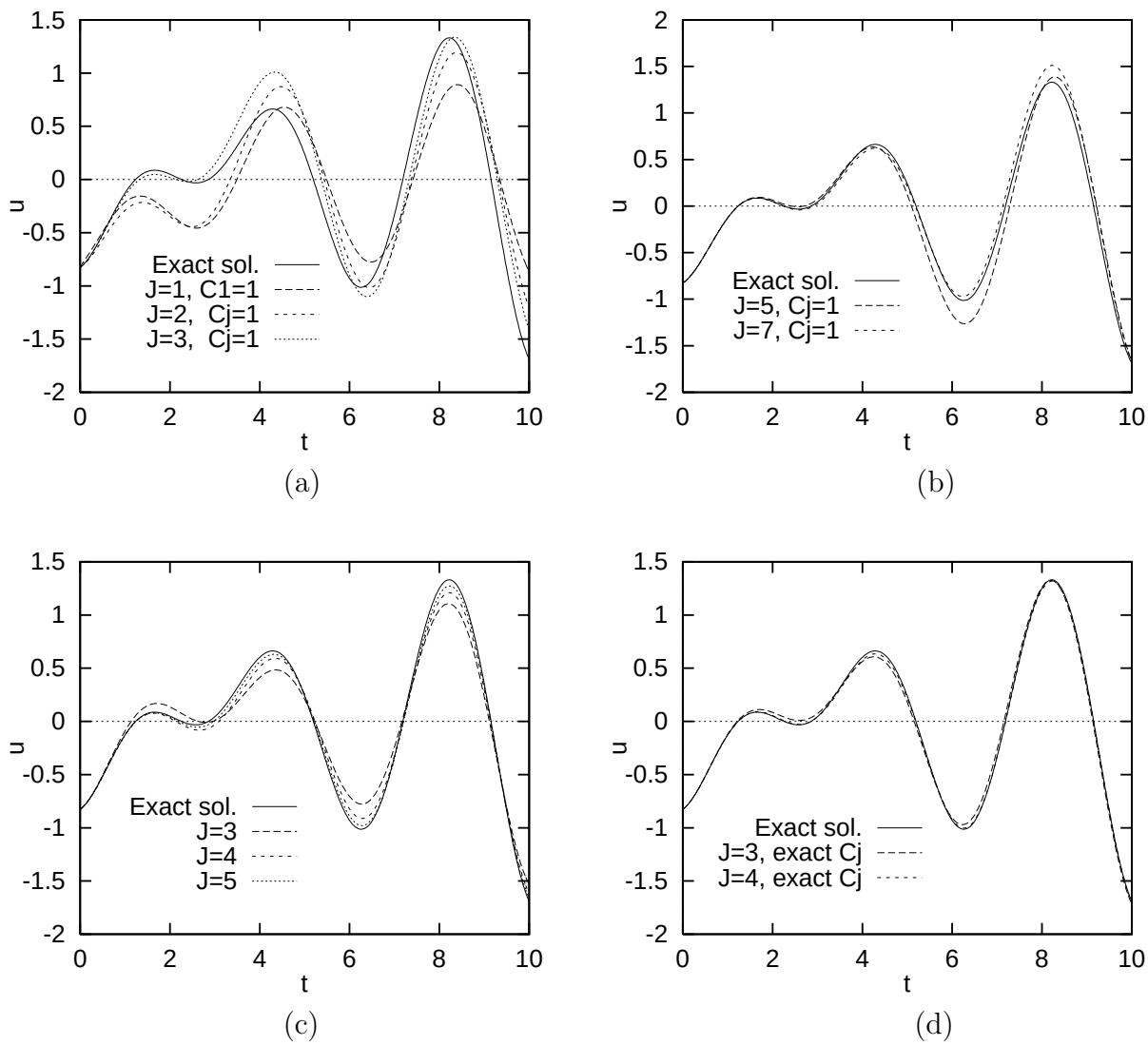

Figure 2: Solution of the three-wave test problem: u at the point $x = 5$, $y = 2.75$ (on Γ_E) as a function of time. (a) Exact solution and the H_1, H_2 and H_3 solutions with $C_j = 1$. (b) Exact solution and the H_5 and H_7 solutions with $C_j = 1$. (c) Exact solution and the H_3, H_4 and H_5 solutions with automatically chosen C_j. (d) Exact solution and the H_3 and H_4 solutions with the exact C_j.

$f = 0.5$. The initial conditions are all zero, and the boundary function u_W on Γ_W is given by

$$u_W(y,t) = \begin{cases} \cos\left[\frac{\pi}{2r}(y-y_0)\right] & \text{if } |y-y_0| \le r \quad \& \quad t \le t_0 \\ 0 & \text{otherwise} \end{cases} \tag{31}$$

Thus, the wave source on the west boundary is a cosine function in y with three parameters: its center location y_0, its width r, and its time duration t_0. We set $y_0 = 2.5$, $r = 1.5$, and $t_0 = 0.5$. In contrast to the previous test problem, the solution of this problem involves an infinite number of modes and frequencies.

The computational parameters x_E, Δt and the grid are the same as in the previous example. However, here we use the Higdon NRBC H_4 on Γ_E, with the four C_j's obtained automatically by using the procedure given in Box 2. These turn out to be $C_j/C_0 = 1$, 3.6, 4.5 and 10.6.

We compare the solution obtained by the new scheme with two other solutions:

- A solution obtained in the same domain, but with the Higdon NRBC H_1 on g_E, using $C_1 = 5$, which in the middle of the range of the four C_j's mentioned above.
- A solution obtained in a domain twice as long, namely the domain $0 \le x \le 10$, $0 \le y \le 5$, using a 42×21 grid with the same resolution. During the simulation time the wave generated on Γ_W does not reach the remote (east) boundary of this large domain, and thus the issue of spurious reflection is avoided altogether, regardless of the boundary condition used on the remote boundary. Hence this will serve as a "reference solution" which is exact as far as the boundary-condition treatment is concerned.

Fig. 3(a) shows the three solutions at time $t = 4$. In this and the next figures, the top plot is that of the reference solution, the middle plot corresponds to the solution obtained by the new scheme with the H_4 NRBC, and the lower plot describes the H_1 solution. Both the colors and the contour lines represent values of u. At time $t = 4$ the main bulk of the wave packet generated on Γ_W has not reached the boundary Γ_E yet, and hence all three plots are similar.

Fig. 3(b) shows the three solutions at time $t = 6$. The wave packet has already passed the boundary Γ_E. The H_4 solution is indistinguishable from the reference solution, whereas in the H_1 solution spurious reflection is evident. Figs. 3(c) and 3(d) correspond to times $t = 8$ and $t = 10$, respectively. The reflected wave moves backwards in the H_1 solution and pollutes the entire computational domain. On the other hand, the H_4 solution exhibits the wave traces which are also present in the reference solution.

Finally we repeat this experiment while increasing the dispersion parameter by a factor of 20, i.e., we take $f = 10$. The group velocity decreases with increasing dispersion; hence the wave packet will move much more slowly now. Also, the solution is expected to be much "richer," being composed of many waves with different frequencies and phase speeds. Indeed, this is seen in Fig. 4(a), which illustrates the solution at time $t = 12.5$. The wave has

just reached the boundary Γ_E, and the beginning of spurious reflection in the H_1 solution is apparent. Figs. 4(b)–(d) show the solutions at times $t = 15$, $t = 19$ and $t = 22.5$, respectively. Again the H_1 solution exhibits spurious reflection, while the H_4 solution performs very well in this high-dispersion case too.

8. Concluding Remarks

In this paper we have presented a new numerical procedure based on FDs, which allows the use of the Higdon NRBCs up to an *arbitrarily high order*. The scheme is coded once and for all for any order; the order of the scheme is simply an input parameter. This adds an important computational tool for use in the solution of infinite domain time-dependent wave problems. Moreover, due to the generality of the Higdon NRBCs it is possible to use this tool for problems with dispersive and layered media. We have focused on dispersive waves in this paper, although the scheme is effective in the non-dispersive case as well. We have demonstrated that the high-order scheme, with the automatically-chosen parameters, performs very well in both the low and high dispersion regimes.

Related future work will include the adaptation of the proposed approach to more complicated configurations, such as exterior problems with a rectangular artificial boundary $\mathcal{B}$, and three-dimensional problems. It should be remarked that no difficulties are expected in the case where $\mathcal{B}$ has *corners*. The Higdon NRBCs do not involve mixed spatial derivatives, and thus the corner grid-point can arbitrarily be associated with one of the two straight edges that meet at this corner, and can be treated just as any other grid point on this chosen edge.

In addition, the high-order Higdon NRBCs will be applied to the Shallow Water Equations (SWEs). The Shallow Water model serves as an important testbed for more complicated models in meteorology [38]. It would be interesting, among other things, to test the performance of the high-order Higdon NRBCs when the *nonlinear* SWEs are used in the computational domain Ω.

An alternative formulation of the Higdon NRBCs is currently under development. In this formulation some auxiliary variables are introduced on the artificial boundary, in order to eliminate all the high-order derivatives. This form of the NRBC has the advantages that after discretization it involves only degrees of freedom on the boundary $\mathcal{B}$ itself, that no high-order discrete schemes are needed, and that the history of the solution does not have to be stored. As a result, it is more amenable, compared to the formulation presented in this paper, for incorporation in a Finite Element scheme. This alternative formulation will be reported in a future publication.

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Captions for Figures

Fig. 1. Setup for the wave-guide problem: (a) the original problem in a semi-infinite wave guide; (b) the computational problem in a finite domain Ω.

Fig. 2. Solution of the three-wave test problem: u at the point $x = 5$, $y = 2.75$ (on Γ_E) as a function of time. (a) Exact solution and the H_1, H_2 and H_3 solutions with $C_j = 1$. (b) Exact solution and the H_5 and H_7 solutions with $C_j = 1$. (c) Exact solution and the H_3, H_4 and H_5 solutions with automatically chosen C_j. (d) Exact solution and the H_3 and H_4 solutions with the exact C_j.

Fig. 3. Solution of the west-source problem, dispersion parameter $f = 0.5$. Top plot — reference solution, middle plot — H_4 solution, lower plot — H_1 solution. Times: (a) $t = 4$, (b) $t = 6$, (b) $t = 8$, (b) $t = 10$.

Fig. 4. Solution of the west-source problem, dispersion parameter $f = 10$. Top plot — reference solution, middle plot — H_4 solution, lower plot — H_1 solution. Times: (a) $t = 12.5$, (b) $t = 15$, (b) $t = 19$, (b) $t = 22.5$.