DISCRETE TRANSPARENT BOUNDARY CONDITIONS FOR WIDE ANGLE PARABOLIC EQUATIONS: FAST CALCULATION AND APPROXIMATION

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This paper is concerned with the efficient implementation of transparent boundary conditions (TBCs) for wide angle parabolic equations (WAPEs) assuming cylindrical symmetry. In [1] a discrete TBC of convolution type was derived from the fully discretized whole–space problem that is reflection–free and yields an unconditionally stable scheme. Since the discrete TBC includes a convolution with respect to range with a weakly decaying kernel, its numerical evaluation becomes very costly for long-range simulations.

As a remedy we construct new approximative transparent boundary conditions involving exponential sums as an approximation to the convolution kernel. This special approximation enables us to use a fast evaluation of the convolution type boundary condition.

This new approach was outlined in detail in [2] for the standard "parabolic" equation.

1. INTRODUCTION

This paper is concerned with a finite difference discretization of *wide angle "parabolic" equations*. These models appear as one–way approximations to the Helmholtz equation in cylindrical coordinates with azimuthal symmetry. In particular we will discuss the efficient implementation of transparent boundary conditions.

In oceanography one wants to calculate the underwater acoustic pressure $p(z,r)$ emerging from a time–harmonic point source located in the water at $(z_s,0)$. Here, $r>0$ denotes the radial range variable, $0<z<z_b$ is the depth variable. The water surface is at $z=0$, and the (horizontal) sea bottom at $z=z_b$. We denote the local sound speed by $c(z,r)$, the density by $\rho(z,r)$, and the attenuation by $\alpha(z,r)\geq 0$. $n(z,r)=c_0/c(z,r)$ is the refractive index, with a reference sound speed c_0. Then the reference wave number is $k_0=2\pi f/c_0$,

where f denotes the (usually low) frequency of the emitted sound.

We consider the *wide–angle "parabolic" equations* (WAPE)

$$\psi_r = ik_0 \left(\frac{p_0 - p_1 L}{1 - q_1 L} - 1 \right) \psi, \qquad r > 0, \tag{1}$$

with real parameters p_0, p_1, q_1. Here, L denotes the *Schrödinger operator*

$$L = -k_0^{-2} \rho \, \partial_z (\rho^{-1} \partial_z) + V(z,r) \tag{2}$$

with the complex valued "potential" $V(z,r) = 1 - N^2(z,r)$. With the choice $p_0 = 1$, $p_1 = 1/2$, $q_1 = 0$ one obtains the *standard "parabolic" equation* (SPE) of Tappert and $p_0 = 1$, $p_1 = 3/4$, $q_1 = 1/4$ gives the *WAPE of Claerbout*.

In practical simulations one is only interested in the acoustic field $\psi(z,r)$ in the water, i.e. for $0 < z < z_b$. While the physical problem is posed on the unbounded z–interval $(0,\infty)$, one wishes to restrict the computational domain in the z–direction by introducing an *artificial boundary* at or below the sea bottom. At the water surface one usually employs a *Dirichlet ("pressure release") BC*: $\psi(z = 0, r) = 0$.

In [3] an *impedance BC* or *transparent boundary condition* (TBC) for the WAPE was derived, which completely solves the problem of restricting the z–domain without changing the physical model: complementing the WAPE (1) with a TBC at z_b allows to recover — on the finite computational domain $0 < z < z_b$ — the exact half–space solution on $0 < z < \infty$.

While TBCs fully solve the problem of cutting off the z–domain for the analytical equation, their numerical treatment (approximation, stability, efficiency) is a delicate question. In [1] so–called *discrete transparent boundary conditions* (DTBCs) were derived for a Crank–Nicolson finite–difference approximation of the WAPE such that the overall scheme is unconditionally stable and as accurate as the discretized half–space problem. However, there remains the question of relatively high computational costs for their implementation.

The paper is organized as follows: In §2 and §3 we review the (discrete) TBC for the WAPE. In Section 4 we sketch our new approach of approximating the DTBC by a discrete sum of exponentials and present an efficient recursion for evaluating these approximate DTBCs. The numerical example of §5 illustrate the efficiency of the proposed method.

2. TRANSPARENT BOUNDARY CONDITIONS

We assume $\rho = \rho(z)$ (vertical density variations) and apply the operator $1 - q_1 L$ to (1):

$$\begin{aligned} &\left[1 - q_1 V + q_1 k_0^{-2} \rho \, \partial_z(\rho^{-1}\partial_z)\right] \psi_r \\ &\qquad = ik_0 \left[p_0 - 1 - (p_1 - q_1) V + (p_1 - q_1) k_0^{-2} \rho \, \partial_z(\rho^{-1}\partial_z)\right] \psi. \end{aligned} \tag{3}$$

As the density is typically discontinuous at the water–bottom interface ($z = z_b$), one requires continuity of the (acoustic) pressure and the normal particle velocity:

$$\psi(z_b-, r) = \psi(z_b+, r), \qquad \frac{\psi_z(z_b-, r)}{\rho_w} = \frac{\psi_z(z_b+, r)}{\rho_b}, \tag{4}$$

where ρ_w is the water density just above the bottom and ρ_b is the constant bottom density.

For the derivation of the following TBC we shall make the two assumptions (strategies to soften these restrictions could be found in [4]): Let the initial data $\psi^I = \psi(z,0)$, which models a point source located at $(z_s,0)$, be supported in the *interior domain* $0 < z < z_b$. Let the bottom region be *homogenous*, i.e. let all physical parameters be constant for $z > z_b$. The *TBC for the WAPE* was derived by Papadakis [3] and slightly generalized in [1]:

$$\psi_z(z_b,r) = \frac{i}{\eta}\frac{\rho_w}{\rho_b}\psi(z_b,r) \;+\frac{\beta}{\eta}\frac{\rho_w}{\rho_b}\int_0^r \psi(z_b,r-\tau)\,e^{i\theta\tau}e^{i\beta\tau}\big[J_0(\beta\tau)-iJ_1(\beta\tau)\big]\,d\tau, \qquad (5)$$

$$\eta = \frac{1}{k_0}\sqrt[+]{\frac{q_1}{\delta_b}}, \quad \delta_b = 1-q_1(1-N_b^2), \quad \beta = -\frac{p_1-p_0q_1}{2q_1}\frac{k_0}{\delta_b}, \quad \theta = \frac{p_1-q_1}{q_1}k_0,$$

where J_0, J_1 denote the Bessel functions of order 0 and 1, respectively. This TBC is non–local in the range r; in range marching algorithms it thus requires storing the bottom boundary data $\psi(z_b,.)$ of all previous range levels. Moreover, the discretization of the TBC (5) is not trivial at all and inadequate discretizations may introduce strong numerical reflections. In the following we will sketch a new approach to remedy this situation. First we present in §3 the discrete TBC which will be approximated by the sum–of–exponential ansatz in §4.

3. DISCRETE TRANSPARENT BOUNDARY CONDITIONS

We consider a Crank–Nicolson finite difference scheme for the WAPE. For simplicity we use the uniform grid points $r_n = nk$, $k = \Delta r$, $z_j = jh$, $h = \Delta z$, (where $J\Delta z = z_b$) and the approximation $\psi_j^{(n)} \sim \psi(z_j,r_n)$, $j \geq 0$, $n \in \mathbb{N}_0$. The discretized WAPE (3) then reads:

$$\begin{aligned}&\big[1-q_1V_j^{(n+\frac12)}+q_1k_0^{-2}\rho_jD^0_{\frac{h}{2}}(\rho_j^{-1}D^0_{\frac{h}{2}})\big]D_k^+\psi_j^{(n)}\\ &\quad= ik_0\big[p_0-1-(p_1-q_1)V_j^{(n+\frac12)}+(p_1-q_1)k_0^{-2}\rho_jD^0_{\frac{h}{2}}(\rho_j^{-1}D^0_{\frac{h}{2}})\big](\psi_j^{(n)}+\psi_j^{n+1})/2, \qquad (6)\end{aligned}$$

with $V_j^{(n+\frac12)} := V(z_j,r_{n+\frac12})$, $D_k^+\psi_j^n = (\psi_j^{n+1}-\psi_j^n)/k$, $D^0_{\frac{h}{2}}\psi_j^n = (\psi^n_{j+\frac12}-\psi^n_{j-\frac12})/h$.

We remark that the depth discretization on the computational interval $[0,z_b]$ can be nonuniform (*e.g. adaptive in range*) without changing our subsequent analysis. Instead of using an ad–hoc discretization of the TBC (5) we constructed in [1] a *discrete TBC* (DTBC) of the fully discretized half–space problem. This strategy solves at no additional computational costs both problems of instabilities and numerical reflections of the *discretized TBC*.

The DTBC for (6) including the density jump is a discrete convolution in range (cf. [1]):

$$\begin{aligned}&(1+iq)\,\frac{\rho_b}{\rho_{eff}}\,\tilde\psi_{J-1}^{(n)}+\big[(1+iq)\big(1-\frac{\rho_b}{\rho_{eff}}\big)-s_0\big]\tilde\psi_J^{(n)}\\ &\qquad= -(1-iq)\,\frac{\rho_b}{\rho_{eff}}\,\tilde\psi_{J-1}^{(n-1)}-(1-iq)\big(1-\frac{\rho_b}{\rho_{eff}}\big)\tilde\psi_J^{(n-1)}+\sum_{m=1}^{n-1}\tilde\psi_J^{(m)}\,s_{n-m}, \qquad (7)\end{aligned}$$

with $q = kq_1/(2k_0)/(p_1-q_1)$ and the convolution coefficients s_n given explicitly in [1] and the *effective density* defined by $\rho_{eff} = (\rho_w+\rho_b)/2$. We proposed to use an *offset grid*, i.e. $z_j = (j+\frac12)h$, $\tilde\psi_j^{(n)} \sim \psi(z_j,r_n)$, $j = -1(1)J$, where the water–bottom interface with the density jump lies between the grid points $j = J-1$ and J.

Using formula (7) for calculations avoids any boundary reflections and it renders the discrete scheme unconditionally stable (just like the underlying Crank–Nicolson scheme). However, the linearly in r increasing numerical effort to evaluate the DTBCs can sharply raise the total computational costs. Note that we need to evaluate just one convolution of (7) at each range step (at the endpoint of the interval $[0, r_n]$). Since the other points of this convolution are not needed, using an FFT is not practical.

The DTBC (7) includes the discrete convolution of the unknown function with a given kernel s_n. Our approach for fast evaluation of this convolution consists of approximating the kernel by a finite sum of exponentials that *decay* with respect to range: this will permit us to use recurrence formulas for the range marching algorithms.

4. APPROXIMATION BY SUMS OF EXPONENTIALS AND FAST EVALUATION

The convolution coefficients s_n appearing in the DTBC (7) can be calculated by an explicit formula (see [1]) and by a *numerical calculation* of the inverse Z–transform, see [2]. In order to derive a fast numerical method to calculate the discrete convolutions in (7) we will approximate the coefficients s_n by the following *sum-of-exponential ansatz*:

$$s_n \approx \tilde{s}_n := \begin{cases} s_n, & n = 0, 1, \ldots, n_0 - 1, \\ \sum_{l=1}^{L} b_l\, q_l^{-n}, & n = n_0, n_0 + 1, \ldots, \end{cases} \tag{8}$$

where $L \in \mathbb{N}$, $n_0 \geq 0$ are fixed number. For practical purposes we shall choose $n_0 = 2$. Evidently, the approximation properties of $\tilde{s}_n$ depend on L and the corresponding set $\{b_l, q_l\}$. We give a deterministic method of finding $\{b_l, q_l\}$ for fixed L. Consider the power series:

$$f(x) := s_{n_0} + s_{n_0+1}x + s_{n_0+2}x^2 + \ldots, \qquad |x| \leq 1. \tag{9}$$

If there exists the $[L-1|L]$ Padé approximation $\tilde{f}(x) := \frac{P_{L-1}(x)}{Q_L(x)}$ of (9), then its Taylor series

$$\tilde{f}(x) = \tilde{s}_{n_0} + \tilde{s}_{n_0+1}x + \tilde{s}_{n_0+2}x^2 + \ldots \tag{10}$$

satisfies the conditions $\tilde{s}_n = s_n$, $n = n_0, n_0+1, \ldots, 2L+n_0-1$, according to the definition of the Padé approximation rule.

Theorem 1 ([2]). *Let $Q_L(x)$ have L simple roots q_l with $|q_l| > 1, \quad l = 1, \ldots, L$. Then*

$$\tilde{s}_n = \sum_{l=1}^{L} b_l q_l^{-n}, \qquad n = n_0, n_0+1, \ldots, \tag{11}$$

$$b_l := -\frac{P_{L-1}(q_l)}{Q_L'(q_l)} q_l^{n_0-1} \neq 0, \qquad l = 1, \ldots, L. \tag{12}$$

We remark that all our practical calculations confirm that the assumption on $Q_L(x)$ in Theorem 1 holds for any desired L, although we cannot prove this.

The set $\{b_l, q_l\}$ can be used in (8) at least for $n = n_0, n_0+1, \ldots, 2L+n_0-1$. The main question is: is it possible to use $\{b_l, q_l\}$ also for $n > 2L+n_0-1$? What quality of approximation $\tilde{s}_n \approx s_n$, $n > 2L+n_0-1$ can one expect?

Although the asymptotic behaviour of s_n and $\tilde{s}_n$ (as $n \to \infty$) differs strongly (algebraic versus exponential decay), the error of the approximation decays exponentially in L (cf. §5).

Let us consider the approximation (8) of the discrete convolution kernel appearing in the DTBC (7). With these "exponential" coefficients the convolution

$$C^{(n)}(\tilde{\psi}_J) := \sum_{m=1}^{n-1} \tilde{s}_{n-m} \tilde{\psi}_J^{(m)}, \quad \tilde{s}_n = \sum_{l=1}^{L} b_l \, q_l^{-n}, \quad |q_l| > 1, \tag{13}$$

of a discrete function $\tilde{\psi}_J^{(m)}$, $m = 1, 2, \ldots$, with the kernel coefficients $\tilde{s}_n$ can be calculated by recurrence formulas. And this will reduce the numerical effort drastically (cf. [2]). The value $C^{(n)}(\tilde{\psi}_J)$ from (13) for $n \geq n_0 + 1$ is represented by $C^{(n)}(\tilde{\psi}_J) = \sum_{l=1}^{L} C_l^{(n)}(\tilde{\psi}_J)$, where

$$C_l^{(n_0)}(\tilde{\psi}_J) \equiv 0, \tag{14}$$

$$C_l^{(n)}(\tilde{\psi}_J) = q_l^{-1} C_l^{(n-1)}(\tilde{\psi}_J) + b_l \, q_l^{-n_0} \tilde{\psi}_J^{(n-n_0)}, \quad n = n_0+1, n_0+2, \ldots. \tag{15}$$

5. NUMERICAL EXAMPLE

We consider the WAPE of Claerbout and the NORDA test case 3B from the PE Workshop I (cf. [1, Example 2]). The environment for this example consists of an isovelocity water column ($c(z) = 1500\,\mathrm{ms}^{-1}$) over an isovelocity half–space bottom ($c_b = 1590\,\mathrm{ms}^{-1}$). The density changes at $z_b = 100\,\mathrm{m}$ from $\rho_w = 1.0\,\mathrm{gcm}^{-3}$ in the water to $\rho_b = 1.2\,\mathrm{gcm}^{-3}$ in the bottom. The source and the receiver are located at the same depth $z_s = z_r = 99.5\,\mathrm{m}$. The source frequency is $f = 250\,\mathrm{Hz}$. The attenuation in the water is zero and the bottom attenuation is $\alpha_b = 0.5\,\mathrm{dB}/\lambda_b$, where $\lambda_b = c_b/f$ is the wavelength of sound in the bottom.

The maximum range of interest is 10 km and the reference sound speed is chosen as $c_0 = 1500\,\mathrm{ms}^{-1}$. The calculations were carried out using the depth step $\Delta z = 0.25\,\mathrm{m}$ and the range step $\Delta r = 2.5\,\mathrm{m}$, i.e. 4000 steps in range. Since the source is placed close to the bottom, the TBC was applied 10 m below the ocean–bottom interface.

In the following Table 1 we show the ℓ^∞-error of the approximated $\tilde{s}_n$ to the exact s_n. We remark that the ℓ^∞-error is the significant quantity in the error estimates in [2].

$L =$	10	20	30	40	50
error $\|\tilde{s}_n - s_n\|_{\ell^\infty}$	5.4386e-04	3.9713e-05	1.0114e-05	9.3090e-07	5.1059e-08

Table 1: Maximum error of approximated convolution coefficients for $n = 1, \ldots, 4000$.

Figure 1 shows the relative L^2-error of the approximate solution ψ_a in the water region defined by $e_L(z,r) := (\psi_a(z,r) - \psi_{ref}(z,r))/||\psi^I||_2$.

6. CONCLUSIONS

We have constructed new approximate TBCs with a kernel having the form of a finite sum–of–exponentials, which can be evaluated efficiently by a simple recursion. This approach will reduce the numerical effort drastically especially for large–range computations.

A much more detailed version of this article (including stability proofs, error estimates and numerical results) will be published elsewhere.

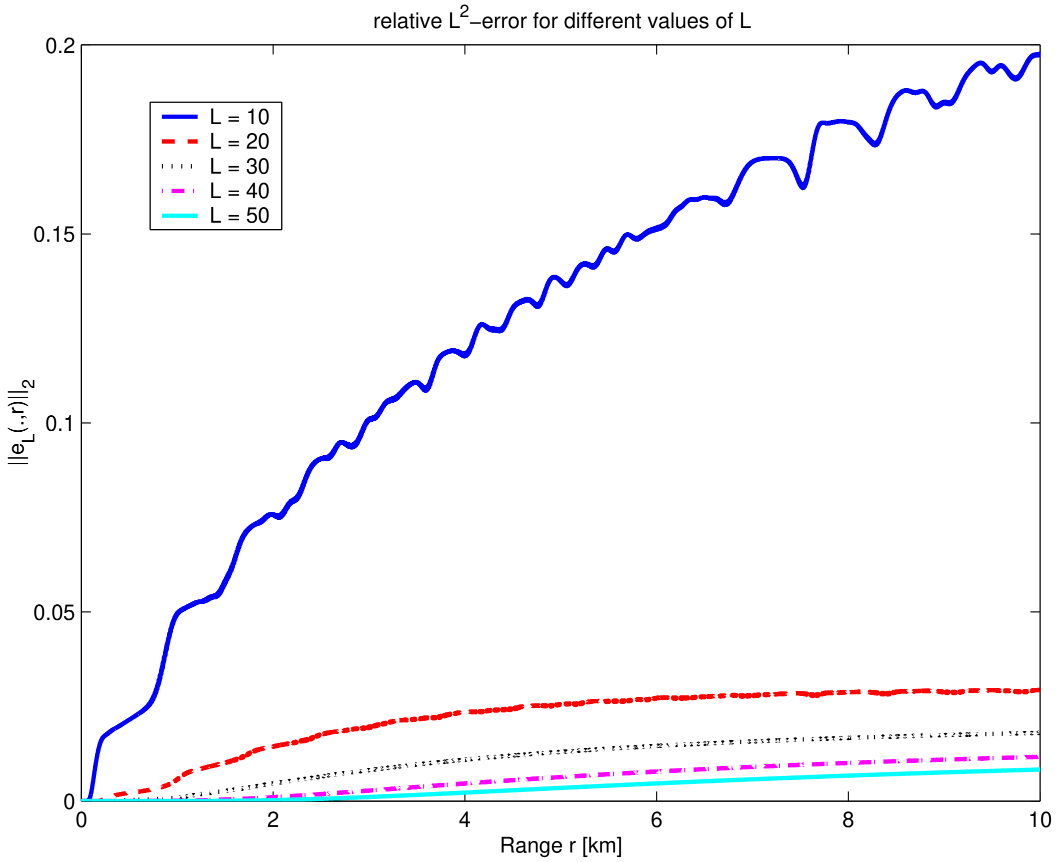

Fig. 1: Relative L^2-error due to approximative TBC.

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