Efficient Numerical Implementation of Discrete Transparent Boundary Conditions for Parabolic Equations

M. Ehrhardt

Universität des Saarlandes, Fakultät für Mathematik und Informatik, Postfach 15 11 50, D-66041 Saarbrücken, Germany, e-mail: ehrhardt@num.uni-sb.de

Summary

This paper is concerned with transparent boundary conditions (TBCs) for wide angle parabolic equations (WAPEs) in the application to underwater acoustics (assuming cylindrical symmetry). These TBCs can be derived for a bottom region in which the squared refractive index is constant or varies linearly with depth. In a previous work 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. However, since the perfect discrete TBC for the WAPE is non–local in range, its numerical evaluation becomes very costly for large–range simulations. As a remedy we construct new approximate TBCs in the form of a discrete sum–of–exponentials, which can be evaluated in a very efficient recursion. Furthermore, we extend the discrete TBC to the case that the starting field is not supported inside the water region (which is the computational domain).

1. Introduction

This paper is concerned with an efficient implementation of transparent boundary conditions (TBCs) for a finite difference discretization of *standard* and *wide angle "parabolic" equations* (see e.g. [10]). These models appear as one–way approximations to the Helmholtz equation in cylindrical coordinates with azimuthal symmetry.

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 and $0<z<z_b$ 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. The reference wave number is $k_0=2\pi f/c_0$, where f denotes the (usually low) frequency of the emitted sound.

In the far field approximation ($k_0 r \gg 1$) the (complex valued) *outgoing acoustic field* $\psi(z,r)=\sqrt{k_0 r}\,p(z,r)\,e^{-ik_0 r}$ satisfies the *one–way Helmholtz equation*:

$$\psi_r = ik_0\big(\sqrt{1-L}-1\big)\psi, \qquad r>0. \tag{1}$$

Here, $\sqrt{1-L}$ is a pseudo–differential operator, and L the *Schrödinger operator*

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

where $N(z,r)=n(z,r)+i\alpha(z,r)/k_0$ denotes the complex refractive index.

"Parabolic" approximations of (1) consist in formally approximating the pseudo–differential operator $\sqrt{1-L}$ by rational functions of L [10]. The linear approximation of $\sqrt{1-\lambda}$ by $1-\lambda/2$ gives the narrow angle or *standard "parabolic" equation* (SPE)

$$\psi_r = -\frac{ik_0}{2}L\psi, \qquad r>0. \tag{3}$$

Rational approximations of the form $\sqrt{1-\lambda}\approx f(\lambda)=(p_0-p_1\lambda)/(1-q_1\lambda)$ with real p_0, p_1, q_1 yield the *wide angle "parabolic" equations* (WAPE)

$$\psi_r = ik_0\left(\frac{p_0-p_1L}{1-q_1L}-1\right)\psi, \qquad r>0. \tag{4}$$

In the sequel we will require $f'(0)=p_0q_1-p_1<0$. With the choice $p_0=1$, $p_1=3/4$, $q_1=1/4$ ((1,1)–Padé approximant of $\sqrt{1-\lambda}$) one obtains the *WAPE of Claerbout*.

In this paper we shall focus on boundary conditions (BCs) for the SPE (3) and the WAPE (4). At the water surface one usually employs a Dirichlet ("pressure release") BC : $\psi(z=0,r)=0$. In the z–direction one wishes to restrict the computational domain by introducing an artificial boundary at or below the sea bottom. In [14] Papadakis derived *impedance BCs* or *transparent boundary conditions* (TBCs) for the SPE and the WAPE: complementing the WAPE (4) with a TBC at z_b allows to recover — on the finite computational domain $(0,z_b)$ — the exact half–space solution on $0<z<\infty$. As the SPE is a Schrödinger equation, similar strategies have been developed independently for quantum mechanical applications (see e.g. [3] and the references therein).

While TBCs fully solve the problem of cutting off the z–domain for the analytical equation, all available numerical discretizations suffer from reduced accuracy (in comparison to the discretized half–space problem) and render the overall numerical scheme only conditionally stable [13, 16]. In [4] *discrete transparent boundary conditions* (DTBCs) for a Crank–Nicolson finite difference discretization of the WAPE were constructed such that the overall scheme is unconditionally stable and as accurate as the discretized half–space problem.

We shall now turn to the main motivation of this paper. As the TBCs, the DTBCs are non–local in r, i.e. in range marching algorithms they thus require storing the bottom boundary data of all previous range levels. The (in r) increasing numerical effort to evaluate the DTBCs can sharply raise the total computational costs. Strategies to overcome this drawback will be the key issue of this paper.

The paper is organized as follows: In §2 and §3 we review different (discrete) TBCs for the SPE and the WAPE. In Section 4 we sketch our new approach of approximating the DTBC by a discrete sum of exponentials, and in §5 we present an efficient recursion for evaluating these approximate DTBCs.

2. Transparent Boundary Conditions

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

$$\psi(z_b-,r)=\psi(z_b+,r),\qquad \frac{\psi_z(z_b-,r)}{\rho_w}=\frac{\psi_z(z_b+,r)}{\rho_b}, \tag{5}$$

where $\rho_w=\rho(z_b-,r)$ and ρ_b denotes the constant density of the bottom.

We assume that the initial data $\psi^I=\psi(z,0)$ which models a point source located at $(z_s,0)$, is supported in the computational domain $0<z<z_b$ and that the bottom region be *homogenous*, i.e. all physical parameters are constant for $z>z_b$ (denoted with a subscript 'b'). The TBC for the SPE (or Schrödinger equation) was derived in [3, 13, 14]:

$$\psi(z_b,r)=\frac{-e^{\frac{\pi}{4}i}}{\sqrt{2\pi k_0}}\frac{\rho_b}{\rho_w}\int_0^r\psi_z(z_b,r-\tau)\frac{e^{ib\tau}}{\sqrt{\tau}}\,d\tau, \tag{6}$$

with $b=k_0(N_b^2-1)/2$.

The TBC at the bottom for the WAPE was derived in [4] and reads:

$$\psi(z_b,r)=-i\eta\frac{\rho_b}{\rho_w}\psi_z(z_b,r)+\beta\eta\frac{\rho_b}{\rho_w}\cdot\int_0^r\psi_z(z_b,r-\tau)\,e^{i(\theta+\beta)\tau}\big[J_0(\beta\tau)+iJ_1(\beta\tau)\big]d\tau, \tag{7}$$

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

with $\delta_b=1-q_1(1-N_b^2)$ and $\sqrt[+]{}$ denotes the branch of the square root with a nonnegative real part. This is a slight generalization of the TBC derived in [14] where p_0 was equal to 1.

If the starting field $\psi^I=\psi(z,0)$ is not supported in $0<z<z_b$. In [11] Levy derived the TBC

$$\psi_z(z_b,r)=\frac{ice^{-ibr}}{\sqrt{\pi}}\frac{\rho_b}{\rho_w}\int_0^r\frac{\psi_r(z_b,\tau)}{\sqrt{r-\tau}}\,d\tau-\frac{ice^{-ibr}}{\sqrt{\pi r}}\frac{\rho_b}{\rho_w}\int_{z_b}^\infty\psi_z^I(z)\,e^{\frac{ik_0(z-z_b)^2}{2r}}\,dz. \tag{8}$$

$c=(1+i)\sqrt{k_0}$. This TBC was derived by Levy in [11] for the potential–free case.

In the case of a *linear squared refractive index* in the bottom:

$$N_b^2(z,r)=1+\beta+\mu(z-z_b), \tag{9}$$

with real parameters β and $\mu\neq0$ (i.e. no attenuation in the bottom: $\alpha_b=0$) the *transparent BC* at $z=z_b$ (cf. [12]) reads:

$$\psi_z(z_b,r)=\int_0^r\psi_r(z_b,r')\,g(r-r')\,dr'. \tag{10}$$

The integral kernel g in (10) is obtained by an inverse Laplace transformation:

$$g(r) = \sigma \left\{ \frac{\mathrm{Ai}'(\xi_0(z_b))}{\mathrm{Ai}(\xi_0(z_b))} + \sum_{j=1}^{\infty} \frac{\exp[(a_j - \xi_0(z_b))r/\tau]}{a_j - \xi_0(z_b)} \right\} \tag{11}$$

where $\xi_0(z_b) = \sigma\beta/\mu$ and the a_j are the zeros of the Airy function Ai which are all located on the negative real axis. The parameter σ is chosen to be

$$\sigma = \begin{cases} (\mu k_0^2)^{1/3} e^{-i\pi/3}, & \mu > 0 \\ (-\mu k_0^2)^{1/3}, & \mu < 0 \end{cases}. \tag{12}$$

Here, $\mu > 0$ corresponds to a downward-refracting bottom (energy loss) and $\mu < 0$ represents the upward-refracting case, i.e. energy is returned from the bottom. We remark that the TBC (10) was used in [7] for underwater acoustics applications.

However, all these TBCs suffer from the fact that they are of memory–type, i.e. their numerical implementation requires to store the boundary data $\psi(z_b,.)$ of all the past ranges. In the following we will sketch our approach to remedy this situation. First we present in §3 the discrete TBCs which will be approximated by sum–of–exponential ansatz in §4.

3. Discrete Transparent Boundary Conditions

With the uniform grid points $z_j = jh$, $r_n = nk$ ($h = \Delta z$, $k = \Delta r$) and the approximation $\psi_j^n \sim \psi(z_j, r_n)$ the *Crank–Nicolson difference scheme* for the WAPE is:

$$\begin{aligned}
&\big[1 - q_1 V_j^{n+\frac{1}{2}} + q_1 k_0^{-2} \rho_j D^0_{\frac{h}{2}} (\rho_j^{-1} D^0_{\frac{h}{2}})\big] D_k^+ \psi_j^n \\
&\quad = i k_0 \big[p_0 - 1 - (p_1 - q_1) V_j^{n+\frac{1}{2}} \\
&\quad + (p_1 - q_1) k_0^{-2} \rho_j D^0_{\frac{h}{2}} (\rho_j^{-1} D^0_{\frac{h}{2}})\big] (\psi_j^n + \psi_j^{n+1})/2,
\end{aligned} \tag{13}$$

with $V_j^{n+\frac{1}{2}} := 1 - N^2(z_j, r_{n+\frac{1}{2}})$, $D_k^+ \psi_j^n = (\psi_j^{n+1} - \psi_j^n)/k$, $D^0_{\frac{h}{2}} \psi_j^n = (\psi_{j+\frac{1}{2}}^n - \psi_{j-\frac{1}{2}}^n)/h$. This scheme is second order in h and k and unconditionally stable. [1].

In [16] Thomson and Mayfield used an *ad–hoc discretization of the analytic TBC* (6) and Mayfield [13] showed that this *discretized TBC* for the SPE destroys the unconditional stability of the underlying Crank–Nicolson scheme and induces numerical reflections at the boundary, particularly when using coarse grids.

Instead of using an ad–hoc discretization of the analytic TBCs we constructed in [4] *discrete TBCs* of the fully discretized half–space problem. This strategy solves at no additional computational costs both problems (stability and accuracy) of the *discretized TBC*.

For simplicity of the presentation we will neglect the density jump at $z = z_b$. The DTBC for the SPE and the WAPE reads:

$$\begin{aligned}
&(1 + iq)\, \psi_{J-1}^n - s_0\, \psi_J^n \\
&\qquad = \sum_{m=1}^{n-1} s_{n-m} \psi_J^m - (1 - iq)\, \psi_{J-1}^{n-1},
\end{aligned} \tag{14}$$

$n \geq 1$, with the convolution coefficients s_n explicitly given in [4] and

$$q = \frac{k}{2} \frac{q_1}{p_1 - q_1} k_0^{-1}. \tag{15}$$

For a discussion of the discrete treatment of the density jump we refer to [4].

The discrete version of the TBC (8) for the SPE ($q = 0$) was derived in [8] :

$$\begin{aligned}
&\psi_{J-1}^n - s_0 \psi_J^n \\
&\qquad = \sum_{m=0}^{n-1} s_{n-m} \psi_J^m - \psi_{J-1}^{n-1} + \sum_{m=1}^{\infty} p_m^{(n)} \varphi_{J+m},
\end{aligned} \tag{16}$$

$n \geq 1$. The inhomogeneity φ_j is given by

$$\varphi_j = \psi_{j+1}^0 - (2 - iR\psi_j^0 + R\kappa_b)\psi_j^0 + \psi_{j-1}^0, \quad j \geq J - 1, \tag{17}$$

$$R = \frac{2k_0}{p_1 - q_1} \frac{h^2}{k}, \tag{18}$$

$$\kappa_b = \frac{k}{2} k_0 \big[p_0 - 1 - (p_1 - q_1)(1 - N_b^2)\big]. \tag{19}$$

The series $(p_m^{(n)})$ is defined by

$$(p_m^{(n)}) := \mathcal{Z}^{-1}\{\nu_1^m(z)\}, \tag{20}$$

where $\nu_1^m(z)$ denotes the solution of

$$\nu^2 - 2\left[1 - \frac{iR}{2} \frac{\delta_b(z-1) - i\kappa_b(z+1)}{z + 1 + iq(z-1)}\right] \nu + 1 = 0. \tag{21}$$

with $|\nu_1(z)| < 1$ and $\delta_b = 1 - q_1(1 - N_b^2)$.

In practical situations the sum (over m) in (16) of course has to be finite (e.g. up to an index $m=M$). This means that the starting field is still compactly supported, but possibly outside of the water region (computational domain). The coefficients $p_m^{(n)}$, $m=1,2,\dots,M$, can be calculated recursively by "continued convolution", i.e.

$$p_1^{(n)} = \mathcal{Z}^{-1}\{\nu_1(z)\}, \qquad p_2^{(n)} = \sum_{k=0}^{n} p_1^{(n-k)} p_1^{(k)},$$
$$p_3^{(n)} = \sum_{k=0}^{n} p_2^{(n-k)} p_1^{(k)}, \quad \text{etc..} \tag{22}$$

Alternatively, since this computation is rather costly, the series $(p_m^{(n)})$ can be calculated by an recursion formula (cf. [8]).

The use of the formulas (14) for calculations permits us to avoid any boundary reflections and it renders the fully discrete scheme unconditionally stable (just like the underlying Crank-Nicolson scheme). However, the (in r) increasing numerical effort to evaluate the DTBCs can sharply raise the total computational costs.

The considered DTBCs (14) include 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 in range marching algorithms, Such kind of trick has been proposed in [15] for the continuous TBC in case of the 3D wave equation and developed in [2] for various hyperbolic problems.

4. Approximation by Sums of Exponentials

In order to derive a fast numerical method to calculate the discrete convolutions in (14) we will approximate the coefficients s_n by the following ansatz (*sum of exponentials*):

$$s_n \approx \tilde{s}_n := \begin{cases} s_n, & n=0 \\ \sum_{l=1}^{L} b_l\, q_l^{-n}, & n=1,2,\dots, \end{cases} \tag{23}$$

where $L \in \mathbb{N}$ is a fixed number. Evidently, the approximation properties of $\tilde{s}_n$ depend on L, and the corresponding set $\{b_l, q_l\}$. Below we propose a deterministic method of finding $\{b_l, q_l\}$ for fixed L.

Let us fix L and consider the formal power series:

$$g(x) := s_1 + s_2 x + s_3 x^2 + \dots, \quad |x| \le 1. \tag{24}$$

If there exists the $[L-1|L]$ *Padé approximation*

$$\tilde{g}(x) := \frac{P_{L-1}(x)}{Q_L(x)} \tag{25}$$

of (24), then its Taylor series

$$\tilde{g}(x) = \tilde{s}_1 + \tilde{s}_2 x + \tilde{s}_3 x^2 + \dots \tag{26}$$

satisfies the conditions

$$\tilde{s}_n = s_n, \qquad n = 1,2,\dots,2L, \tag{27}$$

due to the definition of the Padé approximation rule.

Theorem 1 ([5]) *Let $Q_L(x)$ have L simple roots q_l with $|q_l| > 1$, $\quad l = 1,\dots,L$. Then*

$$\tilde{s}_n = \sum_{l=1}^{L} b_l q_l^{-n}, \qquad n = 1,2,\dots, \tag{28}$$

where

$$b_l := -\frac{P_{L-1}(q_l)}{Q_L'(q_l)} \ne 0, \qquad l = 1,\dots,L. \tag{29}$$

It follows from (27) and (28) that the set $\{b_l, q_l\}$ defined in Theorem 1 can be used in (23) at least for $n = 1,2,..,2L$. The main question now is: is it possible to use these $\{b_l, q_l\}$ also for $n > 2L$? In other words, what quality of approximation

$$\tilde{s}_n \approx s_n, \qquad n > 2L \tag{30}$$

can we expect?

The above analysis permits us to give the following description of the approximation to the convolution coefficients s_n by the representation (23) if we use a $[L-1|L]$ Padé approximant to (24): the first $2L$ coefficients are reproduced exactly, see (27); however, the asymptotic behaviour of s_n and $\tilde{s}_n$ (as $n \to \infty$) differs strongly (algebraic versus exponential decay).

5. Fast Evaluation of the Discrete Convolution

Let us consider the approximation (23) of the discrete convolution kernel appearing in the DTBC (14). With these "exponential" coefficients the convolution

$$C^{(n)} := \sum_{k=1}^{n-1} u_k \tilde{s}_{n-k}, \quad \tilde{s}_n = \sum_{l=1}^{L} b_l\, q_l^{-n}, \tag{31}$$

$|q_l| > 1$, of a discrete function u_k, $k = 1, 2, \ldots$, with the kernel coefficients $\tilde{s}_n$ can be calculated by recurrence formulas. And this will reduce the numerical effort drastically.

A straightforward calculation ([5]) yields: The value $C^{(n)}$ from (31) for $n \geq 2$ is represented by

$$C^{(n)} = \sum_{l=1}^{L} C_l^{(n)}, \tag{32}$$

where

$$C_l^{(1)} \equiv 0,$$

$$C_l^{(n)} = q_l^{-1} C_l^{(n-1)} + b_l\, q_l^{-1} u_{n-1}, \tag{33}$$

$n = 2, 3, \ldots\ l = 1, \ldots, L.$

Finally we summarize the approach by the following algorithm:

1. calculation of $s_n^{(N)}, n = 0, \ldots, N-1$ via explicit representation or numerical inverse Z-transformation
2. calculation of $\tilde{s}_n$ via Padé–algorithm
3. the corresponding coefficients b_l, q_l are used for the calculation of the discrete convolutions

Conclusions and Outlook

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

Since [5] is concerned with the numerical treatment of DTBCs for a finite–difference scheme of the time-dependent 2D–Schrödinger equation (which corresponds to a 3D parabolic equation) we will apply this approach to a 3D SPE/WAPE. Also the discrete version of the TBC (10) is currently under investigation, cf. [9].

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

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