Discrete Transparent Boundary Conditions for Schrödinger–type equations for non–compactly supported initial data

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Abstract

Transparent boundary conditions (TBCs) are an important tool for the truncation of the computational domain in order to compute solutions on an unbounded domain. In this work we want to show how the standard assumption of 'compactly supported data' could be relaxed and derive TBCs for a generalized Schrödinger equation directly for the numerical scheme on the discrete level. With this inhomogeneous TBCs it is not necessary that the initial data lies completely inside the computational region. However, an increased computational effort must be accepted.

Key words: Schrödinger–type equation, transparent boundary condition, unbounded domain, non-compactly supported initial data, finite differences
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1 Introduction

Transparent boundary conditions (TBCs) are an important tool for the truncation of the computational domain in order to compute solutions on an unbounded domain (see the reviews in [10], [11], [25]). In this work we want to show how the standard assumption of *'compactly supported initial data'* could be relaxed and derive inhomogeneous TBCs for a finite difference discretization of so–called *standard* and *wide angle "parabolic" equations* [14]. These models appear as one–way approximations to the Helmholtz equation

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in cylindrical coordinates with azimuthal symmetry and include as a special case the *Schrödinger equation*. With this TBCs it is not necessary that the starting field is completely inside the computational region. This is the case in underwater acoustics if the source is close to the bottom or in radiowave propagation problems when computing coverage diagrams of airborne antennas [15].

In the past two decades *"parabolic" equation* (PE) models have been widely used for wave propagation problems in various application areas, e.g. seismology [6], optics and plasma physics (cf. the references in [5]). Further applications to wave propagation problems can be found in radio frequency technology [22]. Here we will be mainly interested in their application to underwater acoustics, where PEs have been introduced by Tappert [23]. An account on the vast recent literature is given in the survey article [13] and in the book [12]. Thus in the sequel we will use a notation common to the application in underwater acoustics. Nevertheless our approach is generally applicable to all one–way wave propagation problems in 2D.

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 *outgoing acoustic field*

$$\psi(z, r) = \sqrt{k_0 r}\, p(z, r)\, e^{-ik_0 r} \tag{1}$$

satisfies the *one–way Helmholtz equation*:

$$\psi_r = ik_0\Big(\sqrt{1 - L} - 1\Big)\psi, \qquad r > 0. \tag{2}$$

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

$$L = -k_0^{-2}\rho\, \partial_z(\rho^{-1}\partial_z) + 1 - N^2(z, r), \tag{3}$$

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

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

equation (SPE) of Tappert:

$$\psi_r = -\frac{ik_0}{2}\, L\psi, \qquad r > 0. \tag{4}$$

This Schrödinger equation is a reasonable description of waves with a propagation direction within about 15° of the horizontal. 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)

$$\psi_r = ik_0 \left(\frac{p_0 - p_1 L}{1 - q_1 L} - 1 \right) \psi, \qquad r > 0. \tag{5}$$

In the sequel we will repeatedly require $f'(0) = p_0 q_1 - p_1 < 0$. With the choice $p_0 = 1$, $p_1 = 3/4$, $q_1 = 1/4$ $\big((1,1)$–Padé approximant of $\sqrt{1-\lambda}\big)$ one obtains the *WAPE of Claerbout*. If we assume $\rho = \rho(z)$ one can apply the operator $1 - q_1 L$ to (5):

$$\begin{aligned} &\Big[1 - q_1 V + q_1 k_0^{-2} \rho \partial_z (\rho^{-1} \partial_z)\Big] \psi_r \\ &\qquad = ik_0 \Big[p_0 - 1 - (p_1 - q_1) V + (p_1 - q_1) k_0^{-2} \rho\, \partial_z (\rho^{-1} \partial_z)\Big] \psi. \end{aligned} \tag{6}$$

In this paper we shall focus on boundary conditions (BCs) for the SPE (4) and the WAPE (5). 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. Papadakis [20] derived *impedance BCs* (or *TBCs*) for the SPE and the WAPE: complementing the WAPE (5) with a TBC at z_b allows to recover — on the finite computational domain $(0, z_b)$ — the exact half–space solution on $0 < z < \infty$. For an overview paper we refer the reader to [21]. As the SPE is a Schrödinger equation, similar strategies have been developed independently for quantum mechanical applications.

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 [24]. In [3] *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.

In this work we show how to remove one essential restriction of the (discrete) TBCs: we derive (discrete) TBCs for the case that the initial data which models a point source located at $(z_s, 0)$, is not completely contained in the computational domain. However, an increased computational effort must be accepted. While most authors [16], [18] (cf. also Section 8.6 in [14]) use an exterior solution to 'homogenize' the problem, we directly solve the inhomogeneous problem. The usage of this DTBC is especially beneficial when one needs several computations with the same initial data. Then the calculation of the additional term has only to be done once. The same applies when the initial field is concentrated far outside the computational domain. This is the case e.g. in radiowave propagation when computing coverage diagrams of airborne antennas; the (high) source need not be included in the domain and the computation needs far less time.

The paper is organized as follows: In §2 we review the derivation of the continuous TBC and in §3 we derive the discrete TBCs for the SPE and the WAPE. Finally, in §4 we conclude with a numerical example.

2 Transparent Boundary Conditions

In this section we first will derive the continuous *transparent boundary condition* at the sea–bottom interface. For simplicity of the presentation we will restrict ourselves to the TBC for the SPE. The basic idea of the derivation is to explicitly solve the equation in the bottom region, which is the exterior of the computational domain $(0, z_b)$. Therefore we assume that the bottom region is *homogeneous*, i.e. all physical parameters are constant for $z > z_b$ (denoted with a subscript 'b').

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*):

$$\psi(z_b-, r) = \psi(z_b+, r), \qquad \frac{\psi_z(z_b-, r)}{\rho_w} = \frac{\psi_z(z_b+, r)}{\rho_b}, \tag{7}$$

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

In order to derive the TBC we assume that the starting field $\psi^I(z)$ is continuous and consider the SPE (4) in the bottom region:

$$\psi_{zz} + 2ik_0\psi_r - k_0^2\Big(1 - N_b^2\Big)\psi = 0, \quad z > z_b. \tag{8}$$

The Laplace transformation in range of ψ is given by

$$\hat{\psi}(z, s) = \int_0^\infty \psi(z, r)\, e^{-sr}\, dr, \tag{9}$$

where we set $s = \eta + i\xi$, $\xi \in \mathbb{R}$, and $\eta > 0$ is fixed, with the idea to later perform the limit $\eta \to 0$. Now the exterior problem (8) is transformed to

$$\hat{\psi}_{zz} + c^2\Big(s + i\frac{k_0}{2}\big(1 - N_b^2\big)\Big)\hat{\psi} = c^2\psi^I(z), \quad z > z_b, \tag{10}$$

where we set $c = (1+i)\sqrt{k_0}$.

The basic idea is to solve this inhomogeneous second order differential equation (10) explicitly. The homogeneous solution is

$$\hat{\psi}^{hom}(z,s) = C_1(s)\, e^{icq(s)(z-z_b)} + C_2(s)\, e^{-icq(s)(z-z_b)}, \quad z > z_b, \tag{11}$$

with the abbreviation $q(s) = \sqrt[+]{s + ik_0(1-N_b^2)/2}$. A particular solution of (10) is given by

$$\hat{\psi}^{par}(z,s) = \frac{c}{2iq(s)}\left[\int_{z_b}^{z} e^{icq(s)(z-\zeta)}\psi^I(\zeta)\, d\zeta - \int_{z_b}^{z} e^{icq(s)(\zeta-z)}\psi^I(\zeta)\, d\zeta\right], \tag{12}$$

for $z > z_b$, i.e. the *general solution* in the bottom region is

$$\begin{aligned} \hat{\psi}(z,s) &= \hat{\psi}^{hom}(z,s) + \hat{\psi}^{par}(z,s) \\ &= \left[C_1(s)\, e^{-icq(s)z_b} + \frac{c}{2iq(s)}\int_{z_b}^{z} e^{-icq(s)\zeta}\psi^I(\zeta)\, d\zeta\right] e^{icq(s)z} \\ &+ \left[C_2(s)\, e^{icq(s)z_b} - \frac{c}{2iq(s)}\int_{z_b}^{\infty} e^{icq(s)\zeta}\psi^I(\zeta)\, d\zeta \right. \\ &\quad \left. + \frac{c}{2iq(s)}\int_{z}^{\infty} e^{icq(s)\zeta}\psi^I(\zeta)\, d\zeta\right] e^{-icq(s)z}. \end{aligned} \tag{13}$$

Here, $\sqrt[+]{}$ denotes the branch of the square root with nonnegative real part. We note that the last term in (13) is bounded for fixed s and $z \to \infty$. Since the solutions have to decrease as $z \to \infty$, the idea is to eliminate the growing factor $e^{-icq(s)z} = e^{(1-i)\sqrt{k_0}q(s)z}$ by simply choosing

$$C_2(s) = \frac{c}{2iq(s)}\int_{z_b}^{\infty} e^{icq(s)(\zeta-z_b)}\psi^I(\zeta)\, d\zeta. \tag{14}$$

Consequently, we obtain $C_1(s)$ as:

$$C_1(s) = \hat{\psi}(z_b+, s) - \frac{c}{2iq(s)}\int_{z_b}^{\infty} e^{icq(s)(\zeta-z_b)}\psi^I(\zeta)\, d\zeta. \tag{15}$$

From this we get with the matching conditions (7) the following representation of the *transformed TBC*:

$$\begin{aligned} \hat{\psi}_z(z_b-, s) &= ic\frac{\rho_w}{\rho_b}\, q(s)\, C_1(s) - \frac{c^2}{2}\frac{\rho_w}{\rho_b}\int_{z_b}^{\infty} e^{icq(s)(\zeta-z_b)}\psi^I(\zeta)\, d\zeta \\ &= ic\frac{\rho_w}{\rho_b}\, q(s)\, \hat{\psi}(z_b-, s) - c^2\frac{\rho_w}{\rho_b}\int_{z_b}^{\infty} e^{icq(s)(\zeta-z_b)}\psi^I(\zeta)\, d\zeta. \end{aligned} \tag{16}$$

It remains to inverse transform (16). If we further assume that ψ^I is continuously differentiable, then integration by parts yields:

$$\hat{\psi}_z(z_b,s) = \frac{ic}{q(s)}\frac{\rho_w}{\rho_b}\Big[q^2(s)\hat{\psi}(z_b,s) - \psi^I(z_b)\Big] - \frac{ic}{q(s)}\frac{\rho_w}{\rho_b}\int_{z_b}^{\infty} e^{icq(s)(\zeta-z_b)}\psi_z^I(\zeta)\,d\zeta.$$

The inverse Laplace transformation using the convolution theorem gives

$$\begin{aligned}\psi_z(z_b,r) = {} & \frac{ic}{\sqrt{\pi}}\frac{\rho_w}{\rho_b}\int_0^r \frac{\psi_r(z_b,\tau)}{\sqrt{r-\tau}}\,d\tau \\ & - ic\frac{\rho_w}{\rho_b}\mathcal{L}^{-1}\left\{\frac{1}{q(s)}\int_{z_b}^{\infty} e^{icq(s)(\zeta-z_b)}\psi_z^I(\zeta)\,d\zeta\right\}.\end{aligned} \tag{17}$$

Finally, if ψ_z^I is integrable for $z > z_b$, Levy proved [17] that the integration and the inverse Laplace transform can be interchanged in (17) to obtain the *TBC*

$$\psi_z(z_b,r) = \frac{ice^{-ibr}}{\sqrt{\pi}}\frac{\rho_w}{\rho_b}\int_0^r \frac{\psi_r(z_b,\tau)}{\sqrt{r-\tau}}\,d\tau - \frac{ice^{-ibr}}{\sqrt{\pi r}}\frac{\rho_w}{\rho_b}\int_{z_b}^{\infty}\psi_z^I(z)\,e^{\frac{ik_0(z-z_b)^2}{2r}}\,dz, \tag{18}$$

with $b = k_0(N_b^2-1)/2$. This TBC was derived by Levy [17] for the case $N_b = 1$.

Remark 1 *Clearly, if $\psi^I(z) = 0$ for $z > z_b$ then (18) reduces to the well–known TBC derived by Papadakis [19], [20]:*

$$\psi_z(z_b,r) = -\sqrt{\frac{2k_0}{\pi}}\,e^{-\frac{i\pi}{4}}\,e^{ibr}\,\frac{\rho_w}{\rho_b}\,\frac{d}{dr}\int_0^r \frac{\psi(z_b,\tau)\,e^{-ib\tau}}{\sqrt{r-\tau}}\,d\tau. \tag{19}$$

Equivalently, it can be written as

$$\psi(z_b,r) = -\frac{e^{\frac{\pi}{4}i}}{\sqrt{2\pi k_0}}\frac{\rho_b}{\rho_w}\int_0^r \psi_z(z_b,r-\tau)\frac{e^{ib\tau}}{\sqrt{\tau}}\,d\tau. \tag{20}$$

Remark 2 *The results of this section can be extended to the case that the refractive index in the bottom N_b depends on the range r. Using the dephasing function approach [2] (also known as gauge change in quantum mechanics) we introduce in (8) the new variable*

$$\varphi(z,r) = \psi(z,r)\exp\left\{i\frac{k_0}{2}\int_0^r\Big(1-N_b^2(\tau)\Big)\,d\tau\right\}, \quad z > z_b, \tag{21}$$

to get the simple equation

$$\varphi_{zz} + 2ik_0\varphi_r = 0, \quad z > z_b. \tag{22}$$

All these BCs (19), (20) are nonlocal in the range variable r; in range marching algorithms they thus require storing the bottom boundary data of all previous range levels. Also they involve a mildly singular convolution kernel. As motivated in the introduction we will not discretize the continuous TBCs. Instead we will show now how to derive the TBCs on a fully discrete level by mimicking the derivation of the continuous TBC. This approach avoids any unphysical reflections and conserves the stability properties of the underlying finite difference scheme.

3 Discrete Transparent Boundary Conditions

In this section we will present how to derive the discrete TBC for a Crank–Nicolson finite difference scheme for the SPE and the WAPE. Here we shall only consider uniform grids in z and r. While a uniform range discretization is crucial for our construction of discrete TBCs, this construction is independent of the (possibly nonuniform) z–discretization on the interior domain.

For simplicity we consider the uniform grid $z_j = jh$, $r_n = nk$ ($h = \Delta z$, $k = \Delta r$) and the approximation $\psi_j^{(n)} \sim \psi(z_j, r_n)$. The discretized WAPE (6) then reads:

$$\begin{aligned}&\Big[1 - q_1 V_j^{(n+\frac{1}{2})} + q_1 k_0^{-2} \rho_j D_{\frac{h}{2}}^0 (\rho_j^{-1} D_{\frac{h}{2}}^0)\Big] D_k^+ \psi_j^{(n)} \\ &= i k_0 \Big[p_0 - 1 - (p_1 - q_1) V_j^{(n+\frac{1}{2})} + (p_1 - q_1) k_0^{-2} \rho_j D_{\frac{h}{2}}^0 (\rho_j^{-1} D_{\frac{h}{2}}^0)\Big] \frac{\psi_j^{(n)} + \psi_j^{(n+1)}}{2}, \end{aligned} \tag{23}$$

with $V_j^{(n+\frac{1}{2})} := V(z_j, r_{n+\frac{1}{2}})$ and the usual difference operators

$$D_k^+ \psi_j^{(n)} = \frac{\psi_j^{(n+1)} - \psi_j^{(n)}}{k}, \qquad D_{\frac{h}{2}}^0 \psi_j^{(n)} = \frac{\psi_{j+\frac{1}{2}}^{(n)} - \psi_{j-\frac{1}{2}}^{(n)}}{h}.$$

It is well known [1] that this scheme is second order in h and k and unconditionally stable.

To derive the DTBC we will now mimic the derivation of the analytic TBCs from the previous section on a discrete level. We solve the discrete exterior problem in the bottom region, i.e. the Crank–Nicolson finite difference scheme (23) for $j \geq J-1$:

$$\Big[R\delta_b + q\Delta_h^2\Big](\psi_j^{(n+1)} - \psi_j^{(n)}) = i\Big[R\kappa_b + \Delta_h^2\Big](\psi_j^{(n+1)} + \psi_j^{(n)}), \tag{24}$$

with

$$\delta_b = 1 - q_1(1 - N_b^2), \quad R = \frac{2k_0}{p_1 - q_1}\frac{h^2}{k}, \quad q = \frac{2}{k}\frac{q_1}{p_1 - q_1}k_0^{-1},$$
$$\kappa_b = \frac{k}{2}k_0\Big[p_0 - 1 - (p_1 - q_1)(1 - N_b^2)\Big],$$

where $\Delta_h^2 \psi_j^{(n)} = \psi_{j+1}^{(n)} - 2\,\psi_j^{(n)} + \psi_{j-1}^{(n)}$ denotes the second order difference operator, and R is proportional to the parabolic mesh ratio. To solve this difference scheme (24) we use the $\mathcal{Z}$–transform:

$$\mathcal{Z}\{\psi_j^{(n)}\} = \hat{\psi}_j(\zeta) := \sum_{n=0}^{\infty} \psi_j^{(n)}\,\zeta^{-n}, \quad \zeta \in \mathbb{C}, \quad |\zeta| > R_\psi, \tag{25}$$

where R_ψ denotes the convergence radius of this Laurent series. Note that we denoted in (25) the transformation variable with ζ in order to assign z for the depth variable. Thus, the difference equation (24) is transformed to

$$\Delta_h^2 \hat{\psi}_j(\zeta) + iR\frac{\delta_b(\zeta-1) - i\kappa_b(\zeta+1)}{\zeta+1+iq(\zeta-1)}\hat{\psi}_j(\zeta) = \gamma_j\,(\zeta), \quad j \geq J-1, \tag{26}$$

with the inhomogeneity

$$\gamma_j\,(\zeta) = \frac{\zeta}{\zeta+1}\,\Delta_h^2\psi_j^{(0)} + \frac{iR\zeta\big[\delta_b - i\kappa_b\big]}{\zeta+1+iq(\zeta-1)}\psi_j^{(0)}. \tag{27}$$

Equation (26) is an inhomogeneous second order difference equation of the form

$$U_{j+1} + a\,U_j + b\,U_{j-1} = \gamma_j\,, \qquad j \geq J-1. \tag{28}$$

The two linearly independent homogeneous solutions take the form α^j, β^j, $j \geq J$ with $\alpha\beta = b$ and a particular solution (28) can be found with the ansatz of *"variation of constants"*. According to Ehrhardt and Arnold [8] the general solution to the inhomogeneous equation (28) is given by

$$U_j = c\,\alpha^j + d\,\beta^j + \frac{1}{\alpha-\beta}\left[\sum_{m=J}^{j} \alpha^{j-m}\gamma_m - \sum_{m=J}^{j} \beta^{j-m}\gamma_m\right], \quad j \geq J-1, \tag{29}$$

which is the discrete analogue to the solution formula (12) in the continuous case.

Now we use (29) to design a boundary condition at $j = J$. For that purpose we assume $|\alpha| < 1$, $|\beta| > 1$ (recall that $b = \alpha\beta = 1$ for the Crank–Nicolson scheme for solving the wide angle parabolic equation). Proceeding analogously to the continuous case we have to eliminate the growing factor β^j by choosing d appropriately as

$$d = \frac{1}{\alpha-\beta}\sum_{m=J}^{\infty} \beta^{-m}\gamma_m. \tag{30}$$

We obtain from (29)

$$U_j = \left[c + \frac{1}{\alpha-\beta}\sum_{m=J}^{j} \alpha^{-m}\gamma_m\right]\alpha^j + \frac{1}{\alpha-\beta}\sum_{m=j+1}^{\infty} \beta^{j-m}\gamma_m, \quad j \geq J-1. \tag{31}$$

The value of c can be expressed with U_{J-1}:

$$c = \frac{U_{J-1}}{\alpha^{J-1}} - \left(\frac{\beta}{\alpha}\right)^{J-1} \frac{1}{\alpha-\beta} \sum_{m=J}^{\infty} \beta^{-m}\gamma_m,$$

and inserting this into (31) with $j = J$:

$$U_J = c\,\alpha^J + \frac{1}{\alpha-\beta} \sum_{m=J}^{\infty} \beta^{J-m}\gamma_m$$

yields

$$U_J = \alpha\,U_{J-1} - \left(1-\frac{\alpha}{\beta}\right) \frac{1}{\alpha-\beta} \sum_{m=J}^{\infty} \beta^{J-m}\gamma_m = \alpha\,U_{J-1} - \beta^{-1} \sum_{m=0}^{\infty} \beta^{-m}\gamma_{J+m},$$

or equivalently

$$b\,U_{J-1} = \beta\,U_J + \sum_{m=0}^{\infty} b^{-m}\alpha^m\gamma_{J+m}. \tag{32}$$

Finally, we want to apply these results to the discretized WAPE (24) and derive the DTBC at $j = J$ in the situation, when the initial data $\psi_j^{(0)}$ does not vanish for $j \geq J-1$. In this case the *$\mathcal{Z}$–transformed exterior Crank–Nicolson scheme reads*:

$$\hat{\psi}_{j+1}(\zeta) - \left[2 - iR\frac{\delta_b(\zeta-1) - i\kappa_b(\zeta+1)}{\zeta+1+iq(\zeta-1)}\right] \hat{\psi}_j(\zeta) + \hat{\psi}_{j-1}(\zeta) = \gamma_j\,(\zeta), \tag{33}$$

$j \geq J-1$, where the inhomogeneity γ_j is given by (27). An inverse $\mathcal{Z}$-transformation of $\gamma_j(\zeta)$ yields:

$$\gamma_j^{(n)} = \mathcal{Z}^{-1}\left\{\gamma_j(\zeta)\right\} = (-1)^n \Delta_h^2 \psi_j^{(0)} + \frac{iR\big[\delta_b - i\kappa_b\big]}{1+iq} \left(\frac{-1+iq}{1+iq}\right)^n \psi_j^{(0)}. \tag{34}$$

Thus, we can use the general solution formula (32) to obtain the *transformed discrete TBC*:

$$\hat{\psi}_{J-1}(\zeta) = \nu_2(\zeta)\,\hat{\psi}_J(\zeta) + \sum_{m=0}^{\infty} \nu_1^m(\zeta)\,\gamma_{J+m}(\zeta), \tag{35}$$

where ν_1, $\nu_2 = \nu_1^{-1}$ are the two solutions of the quadratic equation

$$\nu^2 - 2\left[1 - \frac{iR}{2}\frac{\delta_b(\zeta-1) - i\kappa_b(\zeta+1)}{\zeta+1+iq(\zeta-1)}\right]\nu + 1 = 0. \tag{36}$$

Remark 3 *Setting $\gamma_j \equiv 0$ (35) reduces to the transformed discrete TBC derived by Arnold and Ehrhardt [3].*

In order to formulate the discrete TBC we define $(p_m^{(n)}) := (1+iq)\mathcal{Z}^{-1}\{\nu_1^m(\zeta)\}$, $m \in \mathbb{N}_0$, and set $(\ell^{(n)}) := (1+iq)\mathcal{Z}^{-1}\{\nu_2(\zeta)\}$. We obtain by inverse transforming (35)

$$(1+iq)\,\psi_{J-1}^{(n)} - \ell^{(0)}\psi_J^{(n)} = \sum_{k=0}^{n-1} \ell^{(n-k)}\psi_J^{(k)} + (1+iq)\,\gamma_J^{(n)} + \sum_{m=1}^{\infty}\sum_{k=0}^{n} p_m^{(k)}\gamma_{J+m}^{(n-k)}, \quad (37)$$

$n \geq 1$, with the convolution coefficients $\ell^{(n)}$ given by

$$\begin{aligned}\ell^{(n)} &= \Big[1 + iq + \frac{i}{2}(\gamma - i\sigma)e^{-i\xi}\Big]\delta_n^0 - \frac{i}{2}H(-1)^n e^{in\xi} \\ &\quad - \zeta\Big\{\widetilde{P}_n(\mu) + e^{-i\xi}\lambda^{-2}\widetilde{P}_{n-1}(\mu) + \omega e^{-i\varphi}\sum_{m=0}^{n-1}(-e^{i\xi})^{n-m}\widetilde{P}_m(\mu)\Big\},\end{aligned} \quad (38)$$

$$\gamma = R\,\delta_b, \quad \sigma = -R\,\kappa_b, \quad \lambda = \sqrt[+]{\frac{E}{G}}, \quad \mu = \frac{F}{\sqrt[+]{EG}}, \quad \omega = \frac{H^2}{|E|},$$
$$\xi = \arg\frac{1-iq}{1+iq}, \quad \varphi = \arg E, \quad \varepsilon = \frac{i}{2}|E|^{\frac{1}{2}}e^{i\frac{\varphi}{2}},$$
$$E = (\gamma + i\sigma)\Big[\gamma - 4q + i(\sigma+4)\Big], \quad F = \gamma(\gamma - 4q) + \sigma(\sigma+4),$$
$$G = (\gamma - i\sigma)\Big[\gamma - 4q - i(\sigma+4)\Big], \quad H = \gamma + i\sigma + (\gamma - i\sigma)e^{-i\xi}.$$

In (38) δ_n^0 denotes the Kronecker symbol and $\widetilde{P}_n(\mu) := \lambda^{-n}P_n(\mu)$ the *damped Legendre polynomials* ($\widetilde{P}_0 \equiv 1$, $\widetilde{P}_{-1} \equiv 0$). In the non–dissipative case ($\alpha_b = 0$) we have $|\lambda| = 1$, $\mu \in [-1,1]$, and hence $|P_n(\mu)| \leq 1$. In the dissipative case $\alpha_b > 0$ we have $|\lambda| > 1$, μ becomes complex and $|P_n(\mu)|$ typically grows with n. In order to evaluate $\ell^{(n)}$ in a numerically stable fashion it is therefore necessary to use the damped polynomials $\widetilde{P}_n(\mu)$ in (38).

The convolution coefficients $\ell^{(n)}$ behave asymptotically as

$$\ell^{(n)} \cong \text{const.}(-1)^n e^{in\xi}, \quad n \to \infty, \quad \xi = \arg\frac{1-iq}{1+iq}, \quad (39)$$

which may lead to subtractive cancellation in (37) (note that $\psi_J^{(n)} \approx \psi_J^{(n+1)}$ in a reasonable discretization). Therefore we introduce the *summed coefficients*

$$s^{(n)} := \ell^{(n)} + e^{i\xi}\ell^{(n-1)}, \quad n \geq 1, \quad s^{(0)} := \ell^{(0)}, \quad (40)$$

which are calculated as

$$s^{(n)} = \Big[(1+iq)e^{i\xi} + \frac{i}{2}(\gamma - i\sigma)\Big]\delta_n^1 + \varepsilon\,\frac{\widetilde{P}_n(\mu) - \lambda^{-2}\widetilde{P}_{n-2}(\mu)}{2n-1}, \quad n \geq 1. \quad (41)$$

Alternatively, they can be calculated directly with the recurrence formula

$$s^{(n)} = \frac{2n-3}{n}\mu\lambda^{-1}s^{(n-1)} - \frac{n-3}{n}\lambda^{-2}s^{(n-2)}, \quad n \geq 3, \quad (42)$$

once $s^{(1)}$, $s^{(2)}$ are computed from (41).

Remark 4 *Using asymptotic properties of the Legendre polynomials one finds $s^{(n)} = O(n^{-3/2})$, $n \to \infty$ which agrees with the decay of the convolution kernel in the differential TBCs like (20).*

Finally, we obtain the *DTBC for non–compactly supported initial data* ($n \geq 1$):

$$(1+iq)\,\psi_{J-1}^{(n)} - s^{(0)}\psi_J^{(n)} = \sum_{k=0}^{n-1} s^{(n-k)}\psi_J^{(k)} - (1-iq)\,\psi_{J-1}^{(n-1)} + 2iq(-1)^n\Delta_h^2\psi_J^{(0)} + \sum_{m=1}^{\infty} p_m^{(0)}\gamma_{J+m}^{(n)} + \sum_{m=1}^{\infty}\sum_{k=0}^{n-1}(p_m^{(k+1)} + e^{i\xi}p_m^{(k)})\gamma_{J+m}^{(n-1-k)}. \tag{43}$$

In practical situations the sum (over m) in (43) of course has to be finite (e.g. up to an index $m = M$). This means that the initial condition is still compactly supported, but possibly outside of the computational interval. The coefficients $p_m^{(n)}$, $m = 1, 2, \ldots, M$, can be calculated recursively by *"continued convolution"*, i.e.

$$p_1^{(n)} = (1+iq)\,\mathcal{Z}^{-1}\left\{\nu_1(\zeta)\right\}, \quad p_2^{(n)} = \sum_{k=0}^{n} p_1^{(n-k)}p_1^{(k)}, \quad p_3^{(n)} = \sum_{k=0}^{n} p_2^{(n-k)}p_1^{(k)}, \text{ etc..} \tag{44}$$

Since this computation is rather costly (even when using fast convolution algorithms with FFTs we seek for another way to calculate $\sum_{m=1}^{\infty}\sum_{k=0}^{n-1}(p_m^{(k+1)} + e^{i\xi}p_m^{(k)})\gamma_{J+m}^{(n-1-k)}$, $n \geq 1$. The key idea is to use (36) for $\nu_1(\zeta)$ in order to construct a recurrence relation for the $p_m^{(n)}$ (w.r.t. m). (36) for $\nu_1(\zeta)$ gives

$$\nu_1^{m+1}(\zeta) = \left[2 - iR\frac{\delta_b(\zeta-1) - i\kappa_b(\zeta+1)}{\zeta+1+iq(\zeta-1)}\right]\nu_1^m(\zeta) - \nu_1^{m-1}(\zeta), \quad m \geq 1. \tag{45}$$

An inverse $\mathcal{Z}$–transformation of the term in the brackets in (45) is

$$\mathcal{Z}^{-1}\left\{[\ldots]\right\} = 2\delta_n^0 - iR\frac{(1+iq)[\delta_b + i\kappa_b]\delta_n^0 - 2[\delta_b + i\kappa_b]\left(\frac{-1+iq}{1+iq}\right)^n}{-1-q^2}, \tag{46}$$

and thus we obtain for $m \geq 1$:

$$p_{m+1}^{(n)} = c_1 p_m^{(n)} - c_2\sum_{k=0}^{n}(-1)^k e^{ik\xi}p_m^{(n-k)} - p_{m-1}^{(n)}, \tag{47}$$

with

$$c_1 = 2(1+iq) + iRe^{-i\xi}[\delta_b + i\kappa_b], \quad c_2 = 2iR[\delta_b + i\kappa_b], \tag{48}$$

and the starting sequences $p_0^{(n)} = \delta_n^0$ and $p_1^{(n)} = (1+iq)\mathcal{Z}^{-1}\{\nu_1(\zeta)\}$, $n \ge 0$. To circumvent the convolution in (47) we consider $q_m^{(n)} := p_m^{(n)} + e^{i\xi} p_m^{(n-1)}$, $p_m^{(-1)} = 0$ and obtain

$$q_{m+1}^{(n)} = c_1 q_m^{(n)} - c_2 p_m^{(n)} - q_{m-1}^{(n)}, \quad m \ge 1, \tag{49}$$

to use in the *DTBC* (43) of the form

$$\begin{aligned}(1+iq)\,\psi_{J-1}^{(n)} - s^{(0)}\psi_J^{(n)} = &\sum_{k=0}^{n-1} s^{(n-k)}\psi_J^{(k)} - (1-iq)\,\psi_{J-1}^{(n-1)} + 2iq(-1)^n \Delta_h^2 \psi_J^{(0)} \\ &+ \sum_{m=1}^{M} p_m^{(0)} \gamma_{J+m}^{(n)} + S_M^{(n)}, \quad n \ge 1,\end{aligned} \tag{50}$$

where

$$S_M^{(n)} := \sum_{m=1}^{M} \sum_{k=1}^{n} q_m^{(k)} \gamma_{J+m}^{(n-k)}, \quad n \ge 1. \tag{51}$$

The calculation of (51) with the aid of the recursion formula (49) is done by the following algorithm

(1) $q_0^{(n)} = (1+iq)\delta_n^0 + (1-iq)\delta_n^1$

(2) $q_1^{(n)} = p_1^{(n)} + e^{i\xi} p_1^{(n-1)} = \tilde{s}^{(n)}$

(3) $S_1^{(n)} = \sum_{k=1}^{n} q_m^{(k)} \gamma_{J+m}^{(n-k)}$

(4) `for` $m = 1, \dots, M-1$ `do`

$\quad q_{m+1}^{(n)} = c_1 q_m^{(n)} - c_2 p_m^{(n)} - q_{m-1}^{(n)}$

$\quad S_{m+1}^{(n)} = S_m^{(n)} + \sum_{k=1}^{n} q_{m+1}^{(k)} \gamma_{J+m+1}^{(n-k)}$

$\quad p_{m+1}^{(0)} = q_{m+1}^{(0)}$

$\quad$ `for` $n = 1, \dots, N$ `do`

$\quad\quad p_{m+1}^{(n)} = q_{m+1}^{(n)} - e^{i\xi} p_{m+1}^{(n-1)}$

$\quad$ `end`

`end`

Here N denotes the maximum time index and $\tilde{s}_J^{(n)}$ the summed coefficients given by (41) but with the other sign in front of 'ε'. The computational effort of the above implementation of the discrete TBC is $\mathrm{O}(M \cdot N)$, i.e. the same effort as when enlarging the computational domain sufficiently.

Alternatively, a *second possible implementation* is to consider the transformed discrete TBC (35) and to calculate numerically the inverse $\mathcal{Z}$–transform of the finite sum once:

$$F^{(n)} = \mathcal{Z}^{-1}\Big\{\hat{F}(\zeta)\Big\} = \mathcal{Z}^{-1}\Big\{(1+iq)\sum_{m=0}^{M}\nu_1^m(\zeta)\,\gamma_{J+m}(\zeta).\Big\} \tag{52}$$

The discrete TBC then reads

$$(1+iq)\,\psi_{J-1}^{(n)} - \ell^{(0)}\psi_J^{(n)} = \sum_{k=0}^{n-1}\ell^{(n-k)}\psi_J^{(k)} + F^{(n)}, \quad n \geq 1, \tag{53}$$

with the coefficient $F^{(n)}$ given by

$$F^{(n)} = \frac{\tau^n}{2\pi}\int_0^{2\pi}\hat{F}(\tau e^{i\varphi})e^{in\varphi}\,d\varphi, \quad n \in \mathbb{N}_0, \quad \tau > 0. \tag{54}$$

Since this inverse $\mathcal{Z}$–transformation cannot be done explicitly, we use a numerical inversion technique based on FFT (details can be found in [8]);

So far we did not consider the (typical) *density jump* at the sea bottom in the discrete TBC (50). In [3] we used an *offset grid*, i.e. $\tilde{z}_j = (j+\frac{1}{2})h$, $\tilde{\psi}_j^n \sim \psi(\tilde{z}_j, r_n)$, $j = -1(1)J$, where the water–bottom interface with the density jump lies between the grid points $j = J-1$ and J. For discretizing the matching conditions in this case one wants to find suitable approximations for ψ and ρ at the interface z_b, $\Psi \sim \psi(z_b)$ and $\rho_{eff} = \rho(z_b)$, such that both sides of the discretized second matching condition (7)

$$\frac{1}{\rho_w}\,\frac{\tilde{\psi}_J^{(n)} - \Psi}{h/2} = \frac{1}{\rho_b}\,\frac{\Psi - \tilde{\psi}_{J-1}^{(n)}}{h/2} \quad \text{are equal to} \quad \frac{1}{\rho_{eff}}\,\frac{\tilde{\psi}_J^{(n)} - \tilde{\psi}_{J-1}^{(n)}}{h}. \tag{55}$$

This approach results in an *effective density* $\rho_{eff} = (\rho_w + \rho_b)/2$ (based on a different derivation this was also used by Collins [7]). At the surface we use instead of $\psi_0^{(n)} = 0$ the offset BC $\tilde{\psi}_0^{(n)} = -\tilde{\psi}_{-1}^{(n)}$.

Finally it remains to reformulate the discrete TBC (50) such that the density jump is taken into account. We rewrite the discretization of the second depth derivative at $j = J$ from (23):

$$h^2\Big[\rho_J\;D^0_{\frac{h}{2}}\Big(\rho_J^{-1}D^0_{\frac{h}{2}}\tilde{\psi}_J^{(n)}\Big)\Big] = \Delta_h^2\tilde{\psi}_J^{(n)} + \Big(1 - \frac{\rho_b}{\rho_{eff}}\Big)\Big(\tilde{\psi}_J^{(n)} - \tilde{\psi}_{J-1}^{(n)}\Big). \tag{56}$$

Comparing the r.h.s. of (56) to (24) we observe that only one additional term appears, and instead of (26) we get

$$\hat{\tilde{\psi}}_{J+1}(\zeta) - \left[1 - iR\,\frac{\delta_b(\zeta-1) - i\kappa_b(\zeta+1)}{\zeta+1+iq(\zeta-1)}\right]\hat{\tilde{\psi}}_J(\zeta) \\ = \frac{\rho_b}{\rho_{eff}}\left(\hat{\tilde{\psi}}_J(\zeta) - \hat{\tilde{\psi}}_{J-1}(\zeta)\right) + \tilde{\gamma}_J(\zeta). \quad (57)$$

with the inhomogeneity

$$\tilde{\gamma}_J(\zeta) = \frac{\zeta}{\zeta+1}\Big[\tilde{\psi}^{(0)}_{J+1} - \tilde{\psi}^{(0)}_J - \frac{\rho_b}{\rho_{eff}}\left(\tilde{\psi}^{(0)}_J - \tilde{\psi}^{(0)}_{J-1}\right)\Big] + \frac{iR\zeta\big[\delta_b - i\kappa_b\big]}{\zeta+1+iq(\zeta-1)}\tilde{\psi}^{(0)}_J. \quad (58)$$

Using $\hat{\tilde{\psi}}_{J+1}(\zeta) = \nu_1(\zeta)\,\hat{\tilde{\psi}}_J(\zeta) - \sum_{m=1}^{\infty}\nu_1^m\tilde{\gamma}_{J+m}(\zeta)$, where $\nu_1(z)$ denotes the solution of (36), and considering the fact that $\nu_1(\zeta) + \nu_1^{-1}(\zeta) - 1$ is equal to the term in the squared brackets in (57) we obtain the $\mathcal{Z}$–transformed discrete TBC:

$$\frac{\rho_b}{\rho_{eff}}\left(\hat{\tilde{\psi}}_J(\zeta) - \hat{\tilde{\psi}}_{J-1}(\zeta)\right) = \hat{\tilde{\psi}}_J(\zeta) - \nu_2(\zeta)\hat{\tilde{\psi}}_J(\zeta) - \sum_{m=0}^{\infty}\nu_1^m\tilde{\gamma}_{J+m}(\zeta). \quad (59)$$

Hence, the *discrete TBC including the density jump* reads

$$(1+iq)\,\frac{\rho_b}{\rho_{eff}}\,\tilde{\psi}^{(n)}_{J-1} + \Big[(1+iq)\Big(1 - \frac{\rho_b}{\rho_{eff}}\Big) - \ell^{(0)}\Big]\tilde{\psi}^{(n)}_J \\ = \sum_{k=0}^{n-1}\ell^{(n-k)}\tilde{\psi}^{(k)}_J + (1+iq)\,\tilde{\gamma}^{(n)}_J + \sum_{m=1}^{\infty}\sum_{k=0}^{n}p^{(k)}_m\tilde{\gamma}^{(n-k)}_{J+m}, \quad n \geq 1, \quad (60)$$

and formulated for the summed coefficients:

$$(1+iq)\,\frac{\rho_b}{\rho_{eff}}\,\tilde{\psi}^{(n)}_{J-1} + \Big[(1+iq)\Big(1 - \frac{\rho_b}{\rho_{eff}}\Big) - s^{(0)}\Big]\tilde{\psi}^{(n)}_J \\ = \sum_{k=0}^{n-1}s^{(n-k)}\tilde{\psi}^{(k)}_J - (1-iq)\,\frac{\rho_b}{\rho_{eff}}\,\tilde{\psi}^{(n-1)}_{J-1} - (1-iq)\Big(1 - \frac{\rho_b}{\rho_{eff}}\Big)\tilde{\psi}^{(n-1)}_J \\ + 2iq(-1)^n\Delta_h^2\tilde{\psi}^{(0)}_J + \sum_{m=1}^{\infty}p^{(0)}_m\tilde{\gamma}^{(n)}_{J+m} + \sum_{m=1}^{\infty}\sum_{k=1}^{n}q^{(k)}_m\tilde{\gamma}^{(n-k)}_{J+m}. \quad (61)$$

with the coefficients $s^{(n)}$ given by (41). Setting $\rho_b = \rho_{eff}$ this discrete TBC (61) reduces to (43).

4 Numerical Example

In this Section we present a simple model example to illustrate the numerical results when using our new discrete TBC for the SPE (4). We use an initial field, that is partially outside the computational domain. Due to its construction, our DTBC yields exactly (up to round–off errors) the numerical whole–space solution restricted to the computational interval $[0, z_b]$.

Example 1 *This example shows a simulation of a right travelling Gaussian beam* $[\psi^I(z) = \exp(i100z - 30(z-0.8)^2)]$ *at three consecutive times evolving under the SPE with* $N^2 \equiv 1$ $(k_0 = 1)$ *and with the rather coarse depth discretization of 161 grid points for the interval* $0 \le z \le 1$ *(i.e.* $\Delta z = 1/160$*) and the range step* $\Delta r = 2 \cdot 10^{-5}$*. For the exterior (computational) domain we choose the same depth step* Δz *and use 60 grid points which results in the exterior interval* $1 < z \le 1.38125$*.*

In the following Fig. 1 we plotted the absolute value of the initial data and the solution obtained with the discrete TBCs (43) at the range steps $r = 0.002$*,* $r = 0.004$*,* $r = 0.006$*. One clearly sees in Fig. 1 that the solution is solely propagated to the right and no artificial reflections are caused.*

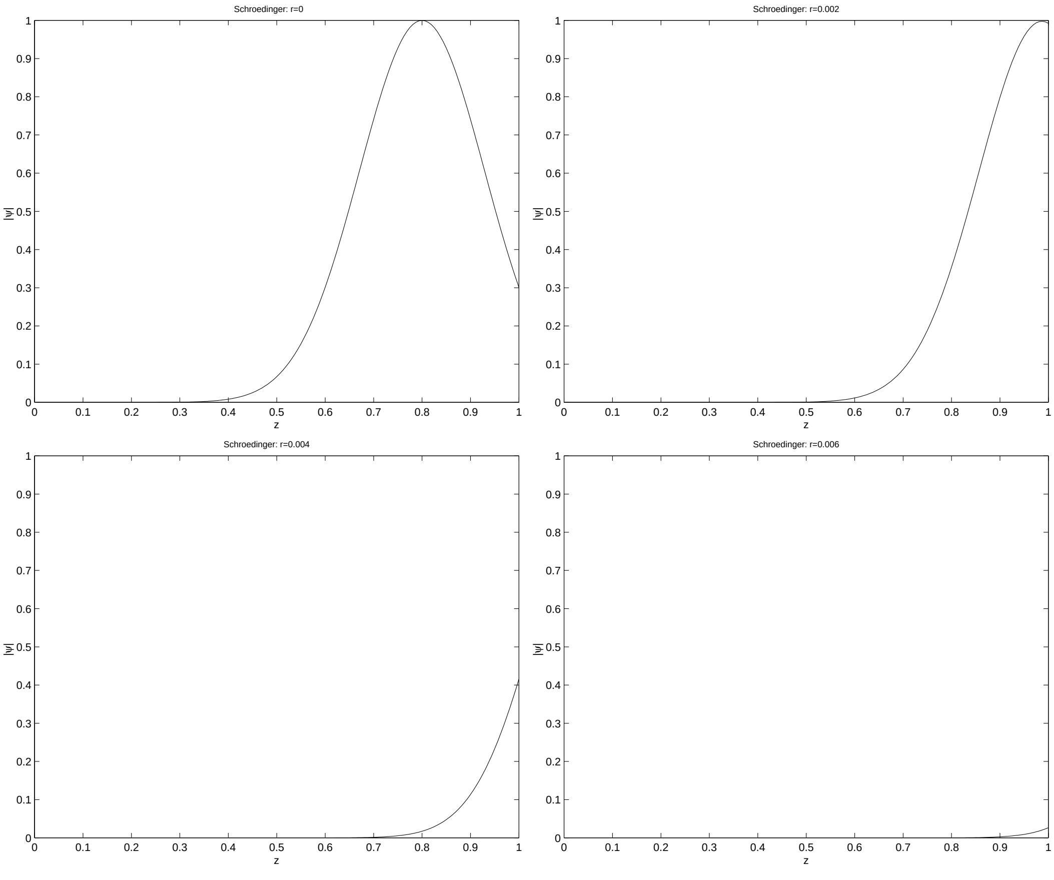

Fig. 1. Solution $|\psi(z,r)|$ at range $r = 0$, $r = 0.002$, $r = 0.004$, $r = 0.006$: the solution with the new discrete TBCs (43) coincides with the whole–space solution and does not introduce any numerical reflections.

In this example the computation using the inhomogeneous DTBCs (50) needs approximately the same CPU–time than just enlarging the domain to the in-

terval $0 \leq z \leq 1.8$ *using a simple Neumann boundary condition at* $z = 1.8$*. From Fig. 1 one can guess that the solution at* $r = 0.004$ *has already reached the boundary at* $z = 1.8$*. Hence it is worthwhile in this example to use the inhomogeneous DTBCs whenever the solution for* $r > 0.004$ *is needed.*

5 Conclusion

We have derived discrete transparent boundary conditions for starting fields that are (partially) supported outside of the computational domain. While the discrete TBC solves the problem of cutting off the computational domain, the resulting numerical effort of this approach is not completely settled yet and subject to further investigations. In particular one has to compare an "optimal" computation algorithm for the coefficients $p_n^{(m)}$or $q_n^{(m)}$ with simulations on a sufficiently enlarged computational domain. In a subsequent paper we will introduce a suitable approximation to the the discrete convolutions appearing in the inhomogeneous DTBC (61) in the spirit of the ideas in [4], [9].

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