Nonlocal Boundary Conditions for Higher–Order Parabolic Equations

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This work deals with the efficient numerical solution of the two–dimensional one–way Helmholtz equation posed on an unbounded domain. In this case one has to introduce artificial boundary conditions to confine the computational domain. Here we construct with the $\mathcal{Z}$–transformation so–called discrete transparent boundary conditions for higher–order parabolic equations schemes. These methods are Padé "Parabolic" approximations of the one–way Helmholtz equation and frequently used in integrated optics and (underwater) acoustics.

1 Introduction

In this work we study a numerical method for two–dimensional scalar wave propagation problems which are usually modeled by the Helmholtz equation posed on an unbounded domain in $\mathbb{R}^2$. Typical applications are integrated optics, seismology and underwater acoustics. Generally the full Helmholtz equation in $\mathbb{R}^2$ is solved as a boundary value problem with radiation boundary conditions. However, often one can distinguish a main propagation direction and factorize the Helmholtz equation if the wavenumber is assumed to be constant. Different one–way approximations yield various so–called *Beam Propagation Methods (BPM)* in optics or *Parabolic Equation (PE)* methods in (underwater and aero) acoustics. 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 *underwater acoustics* one wants to calculate the underwater acoustic pressure $p(z,r)$ emerging from a time–harmonic point source of time dependence $\exp(-i2\pi ft)$ located in the water at $(z_s,0)$. Here, $r>0$ denotes the radial range variable, $0<z<z_b$ the depth variable and f denotes the (usually low) frequency of the emitted sound. 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.

We start our considerations with the *Helmholtz equation* for a variable–density medium and a time–harmonic point source

$$\frac{1}{r}\,\frac{\partial}{\partial r}\left(r\,\frac{\partial p}{\partial r}\right)+\rho\,\frac{\partial}{\partial z}\left(\rho^{-1}\,\frac{\partial p}{\partial z}\right)+k_0^2N^2p=0,\qquad r>0, \tag{1}$$

with the *refractive index* $N(z,r)=n(z,r)+i\alpha(z,r)/k_0$, and the reference wave number $k_0=2\pi f/c_0$. In the *far–field approximation* ($k_0r\gg 1$) the *outgoing acoustic field* $\psi(z,r)=\sqrt{k_0r}\,p(z,r)\,e^{-ik_0r}$ satisfies the *one–way Helmholtz equation*:

$$\psi_r=ik_0\big(-1+\sqrt{1-L}\big)\psi,\quad r>0\qquad\text{with}\qquad L=-k_0^{-2}\rho\,\partial_z(\rho^{-1}\partial_z)+V(z,r). \tag{2}$$

Here, $\sqrt{1-L}$ is a pseudo–differential operator, and L the *Schrödinger operator* with the *potential* $V(z,r)=1-N^2(z,r)$.

2 The Higher–Order Parabolic Equations

An efficient solution method for (2) are *Higher–order PEs*; these *Padé "Parabolic" approximations* of the one–way Helmholtz equation (2) formally approximate the pseudo–differential operator $\sqrt{1-L}$ by a (ℓ,m)–Padé approximant:

$$\psi_r=ik_0\Big(\frac{P_\ell(L)}{Q_m(L)}-1\Big)\psi,\qquad r>0,\quad\text{with}\quad\sqrt{1-\lambda}\approx\frac{p_0-p_1\lambda+p_2\lambda^2-...+p_\ell\lambda^\ell}{1-q_1\lambda+q_2\lambda^2-...+q_m\lambda^m}=:\frac{P_\ell(\lambda)}{Q_m(\lambda)}. \tag{3}$$

This approach yields a PDE that is easier to discretize than the pseudo–differential equation (2).

In this paper we shall focus on adequate boundary conditions (BCs) at the sea–bottom for finite difference discretizations of equations of the form (3). At the free water surface one usually employs a Dirichlet ("pressure release") BC: $\psi(z=0,r)=0$. At the sea bottom the wave propagation in water has to be coupled to the wave propagation in the sediments of the bottom. The bottom will be modeled as the homogeneous half–space region $z>z_b$ with constant parameters c_b, ρ_b, and α_b.

First we discretize in range using an *implicit midpoint* discretization with $\psi^n(z)\sim\psi(z,r_n)$, where $r_n=nk$, ($k=\Delta r$):

$$\Big(1+\frac{ik_0}{2}k\big(1-\sqrt{1-L}\big)\Big)\psi^{n+1}(z)=\Big(1-\frac{ik_0}{2}k\big(1-\sqrt{1-L}\big)\Big)\psi^n(z),\quad n\geq 0. \tag{4}$$

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Now using the Padé approximant (3) of the square root operator, (4) can be written as the *semi–discrete evolution equation*

$$\psi^{n+1}(z) = \frac{U^+(L)}{U^-(L)}\,\psi^n(z), \quad U^\pm(L) = \bigl(1 \mp \frac{ik_0}{2}k\bigr)Q_m(L) \pm \frac{ik_0}{2}kP_\ell(L), \quad \deg(U^\pm) = p = \max(\ell, m). \quad (5)$$

To prevent high powers of L we consider a *multiplicative splitting* and write (5) (involving only first powers of L) in the form:

$$\psi^{n+1}(z) = \frac{c_{U^+}}{c_{U^-}} \prod_{l=1}^{p} \frac{1 - a_l L}{1 - b_l L}\,\psi^n(z), \quad n \geq 0. \quad (6)$$

Finally, to solve (6) numerically it remains to discretize the operator L w.r.t. the depth variable z (denoted by L_h, $h = \Delta z$):

$$L_h\psi_j^n = -k_0^{-2}\rho_j D^0_{\frac{h}{2}}(\rho_j^{-1}D^0_{\frac{h}{2}})\psi_j^n + V_j^n\psi_j^n, \qquad D^0_{\frac{h}{2}}\psi_j^n = \frac{\psi^n_{j+\frac12} - \psi^n_{j-\frac12}}{h}, \quad \psi_j^n \sim \psi^n(z_j), \quad z_j = jh. \quad (7)$$

3 The Discrete Transparent Boundary Conditions

The *discrete transparent boundary conditions* (DTBCs) are obtained by a $\mathcal{Z}$–transformation of the fully discrete numerical scheme in the (homogeneous) fluid bottom region $j \geq J$. We make the basic assumptions that the initial data ψ^I, is confined in the computational domain, i.e. $\operatorname{supp}\psi^I \subset (0, z_b)$ and that all physical parameters are constant for $z > z_b$: $\rho = \rho_b$, $V = V_b$.

To derive the DTBC we consider (6) with L replaced by L_h from (7) in the exterior domain ($j \geq J$) and apply the $\mathcal{Z}$–*transformation* $\mathcal{Z}\{\varphi_j^n\} = \hat\varphi_j(\zeta) := \sum_{n=0}^{\infty}\zeta^{-n}\varphi_j^n$, $\zeta \in \mathbb{C}$, $|\zeta| > R_{\hat\varphi_j}$, to the exterior scheme and obtain a discrete system of p second order difference equations (Δ_h^+, Δ_h^- denote the standard forward and backward differences with stepsize h):

$$\mathbf{X}\Delta_h^+\Delta_h^-\hat{\boldsymbol\psi}_j = \mathbf{Y}\hat{\boldsymbol\psi}_j, \quad j \geq J, \qquad \text{with} \quad \hat{\boldsymbol\psi}_j := (\hat\psi, \hat\varphi_1, \ldots, \hat\varphi_{p-1})_j^\top \in \mathbb{C}^p \quad (8)$$

and the matrices $\mathbf{X}$, $\mathbf{Y} \in \mathbb{C}^{p\times p}$. By introducing $\hat{\boldsymbol\xi}_j := \Delta_h^-\hat{\boldsymbol\psi}_j$ we rewrite (8) as a system of 2p first order difference equations

$$\underbrace{\begin{pmatrix}\mathbf{0} & \mathbf{X}\\ \mathbf{I} & -\mathbf{I}\end{pmatrix}}_{\mathbf{A}}\Delta_h^+\begin{pmatrix}\hat{\boldsymbol\psi}_j\\ \hat{\boldsymbol\xi}_j\end{pmatrix} = \underbrace{\begin{pmatrix}\mathbf{Y} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{pmatrix}}_{\mathbf{B}}\begin{pmatrix}\hat{\boldsymbol\psi}_j\\ \hat{\boldsymbol\xi}_j\end{pmatrix}, \quad \text{i.e.} \quad \begin{pmatrix}\hat{\boldsymbol\psi}_{j+1}\\ \hat{\boldsymbol\xi}_{j+1}\end{pmatrix} = (\mathbf{A}^{-1}\mathbf{B} + \mathbf{I})\begin{pmatrix}\hat{\boldsymbol\psi}_j\\ \hat{\boldsymbol\xi}_j\end{pmatrix}, \quad j \geq J\,. \quad (9)$$

We split the Jordan form $\mathbf{J} = \operatorname{diag}(\mathbf{J_1}, \mathbf{J_2})$ of $\mathbf{A}^{-1}\mathbf{B} + \mathbf{I}$ in (9): $\mathbf{J}_1 \in \mathbb{C}^{p\times p}$ containing the Jordan blocks corresponding to solutions decaying for $j \to \infty$ and $\mathbf{J}_2 \in \mathbb{C}^{p\times p}$ those which increase. With the matrix of left eigenvectors $\mathbf{P}^{-1} = \left(\begin{smallmatrix}\mathbf{P}_1 & \mathbf{P}_2\\ \mathbf{P}_3 & \mathbf{P}_4\end{smallmatrix}\right)$

$$\mathbf{P}^{-1}\begin{pmatrix}\hat{\boldsymbol\psi}_{j+1}\\ \hat{\boldsymbol\xi}_{j+1}\end{pmatrix} = \mathbf{P}^{-1}(\mathbf{A}^{-1}\mathbf{B}{+}\mathbf{I})\begin{pmatrix}\hat{\boldsymbol\psi}_j\\ \hat{\boldsymbol\xi}_j\end{pmatrix} = \mathbf{P}^{-1}\mathbf{P}\begin{pmatrix}\mathbf{J}_1 & \mathbf{0}\\ \mathbf{0} & \mathbf{J}_2\end{pmatrix}\begin{pmatrix}\mathbf{P}_1 & \mathbf{P}_2\\ \mathbf{P}_3 & \mathbf{P}_4\end{pmatrix}\begin{pmatrix}\hat{\boldsymbol\psi}_j\\ \hat{\boldsymbol\xi}_j\end{pmatrix} = \begin{pmatrix}\mathbf{J}_1 & \mathbf{0}\\ \mathbf{0} & \mathbf{J}_2\end{pmatrix}\begin{pmatrix}\mathbf{P}_1\hat{\boldsymbol\psi}_j + \mathbf{P}_2\hat{\boldsymbol\xi}_j\\ \mathbf{P}_3\hat{\boldsymbol\psi}_j + \mathbf{P}_4\hat{\boldsymbol\xi}_j\end{pmatrix}$$

holds and the *transformed DTBC* reads $\mathbf{P}_3\hat{\boldsymbol\psi}_J + \mathbf{P}_4\hat{\boldsymbol\xi}_J = 0$. For a regular $\mathbf{P}_4$ the transformed DTBC can be written in *Dirichlet-to-Neumann form* $\Delta_h^-\hat{\boldsymbol\psi}_J = \widehat{\mathbf{D}}\hat{\boldsymbol\psi}_J$, where $\widehat{\mathbf{D}} = -(\mathbf{P}_4)^{-1}\mathbf{P}_3$. Finally, an inverse $\mathcal{Z}$–transformation yields the *DTBC*

$$\boldsymbol\psi_J^{n+1} - \boldsymbol\psi_{J-1}^{n+1} - \mathbf{D}^0\boldsymbol\psi_J^{n+1} = \sum_{l=1}^{n}\mathbf{D}^{n+1-l}\boldsymbol\psi_J^l, \qquad \mathbf{D}^n = \mathcal{Z}^{-1}\{\widehat{\mathbf{D}}(z)\} = \frac{\tau^n}{2\pi}\int_0^{2\pi}\widehat{\mathbf{D}}(\tau e^{i\varphi})e^{in\varphi}\,d\varphi. \quad (10)$$

where the convolution coefficients D^n given by the above Cauchy integral formula.

Remark 3.1 Let us remark that similar approaches are by Mikhin [2] and a *semi–discrete TBC* by Schmidt et al. [3].

We emphasize the fact that, due to its construction, our DTBC (10) yields exactly (up to round–off errors and evanescent errors in the numerical inverse $\mathcal{Z}$–transformation) the numerical solution on the unbounded domain restricted to the finite computational interval. Several numerical examples [1] of higher–order PE approximants to the one–way Helmholtz equation (including the split–step Padé algorithm of Collins) in the application to optics and underwater acoustics illustrates the superior numerical results when using the DTBC (10). We refer the reader to [1] for a much more detailed version of this paper.

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