

# APPROACHES FOR AUTOMATING UNDERWATER SIMULATIONS BY PE METHOD

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#### Abstract

Modern Parabolic Equation (PE) models are capable of rapid and accurate predictions of underwater propagation. To achieve this goal they require not only highquality environmental data but also properly set model parameters, usually selected by a skillful practicing modeler. Automated simulation systems cannot rely on user skills and have to select their parameters through some heuristics. Commonly, the system designers choose a cautious approach and use conservative parameter settings, thus, sacrificing performance for accuracy. This paper examines possible approaches to simplify parameter selection. The paper is focused on using Nonlocal Boundary Conditions (NLBCs) to remove the user-defined parameters related to truncating the computational domain, the so-called "absorbing sponge". In special cases, this approach allows additional speed-up of simulations through pre-computation of sound propagation in horizontally-independent medium layers.

### 1. INTRODUCTION

Underwater sound propagation can be approximately described by the One-Way Wave Equation (OWWE) [3], which is a class of PE. For 2D problems with Cartesian coordinates x (range) and z (depth), OWWE is

$$\frac{\partial}{\partial x} \left[ \rho^{-1/2} \hat{\mathbf{G}}_2 \Psi \right] = i k_0 \rho^{-1/2} \hat{\mathbf{G}} \hat{\mathbf{G}}_2 \Psi \,. \tag{1}$$

Here,  $\Psi$  is the complex pressure envelope,  $k_0 = \omega c_0^{-1}$  is the reference wave number,  $c_0$  is the reference sound speed,  $\rho$  is the medium density,  $\omega = 2\pi f$ , and f is the sound frequency. The sources and current-related terms are omitted for brevity. The operators in Eq. (1) are  $\hat{\mathbf{G}} = (1 + \hat{\mathbf{X}})^{1/2} - 1$ ,  $\hat{\mathbf{G}}_2 = (1 + \hat{\mathbf{X}})^{1/4}$ , and

$$\hat{\mathbf{X}} = \frac{1}{k_0^2} \left\{ \rho \frac{\partial}{\partial z} \left[ \frac{1}{\rho} \frac{\partial}{\partial z} \right] + k^2 - k_0^2 \right\},\tag{2}$$

where  $k = \omega c^{-1}$  is the wavenumber and c is the sound speed. The numerical solution of OWWE [6] is obtained at  $x_n = n\Delta x$  by recursively solving the system of equations

$$U^{n,l} = \rho^{-1/2} \left[ 1 + w_l \hat{\mathbf{X}} \right] \Theta^{n,l}, U^{n,l+1} = \rho^{-1/2} \left[ 1 + \dot{w}_l \hat{\mathbf{X}} \right] \Theta^{n,l}.$$
 (3)

Here,  $U^{n,l}$ , l = 0, ..., L-1, is the energy flux on the  $l^{\text{th}}$  partial step of the  $n^{\text{th}}$  complete step of the PE;  $U^{n,0} = U^n$  and  $U^{n,L} = U^{n+1}$ . Complex coefficients  $w_l$ ,  $\dot{w}_l$  appear from the Padé approximation of the exponent of operator  $\hat{\mathbf{G}}$  [5]; they depend on the range step  $\Delta x$ . The quantities  $\Theta^{n,l}$  are called partical pressures and play important role in calculating the acoustic pressure  $\Psi$  as well as in analysis of energy conservation and reciprocity relationships [6]. Equations (3) are discretized in depth on a uniform grid  $z_j = j\Delta z$  according to Eq. (7[5]).

Unattended PE simulations require automatic choice of the order of Padé approximation L, and range and depth steps  $\Delta x$ ,  $\Delta z$ . In addition, the computational domain must be truncated at some j = N in such a way that approximates the radiation conditions for the field in an unbounded medium. Usually, PE models implement the radiation condition by appending an absorbing layer to the medium and setting the field to zero at the opposite boundary of the layer [4]. This technique results in the increased computational domain, hence, time, and introduces additional adjustable parameters such as the attenuation and thickness of the absorber. This paper focuses on removing the last group of parameters altogether by replacing the artificial absorber with an appropriate set of Nonlocal Boundary Conditions (NLBCs) [7, 2] at the domain boundaries. The NLBC approach is further extended as a general pre-computation technique for layered media. The manuscript presents theoretical results, deferring numerical examples to the presentation.

## 2. EXACT DISCRETE RADIATION NLBCS

The exact discrete NLBCs for OWWE were obtained by Mikhin [5] using Z transformation of the discrete PE in a homogeneous medium. The radiation NLBC at a (virtual) interface in a homogeneous medium is given by Eq. (15) of  $[5]^{\dagger}$ :

$$\boldsymbol{\vartheta}_{J+1} = \boldsymbol{R}\boldsymbol{M}\boldsymbol{R}^{-1}\boldsymbol{\vartheta}_{J} = \boldsymbol{T}(\zeta)\boldsymbol{\vartheta}_{J}\,. \tag{4}$$

Here,  $\boldsymbol{\vartheta}_j = (\vartheta_j^0, \dots, \vartheta_j^{L-1})^T$ , where  $\vartheta_j^l$  is a Z transform of the  $l^{\text{th}}$  partial pressure  $\Theta_j^{l,n}$  at the depth node *j* defined according to Eq. (8[5]);  $\boldsymbol{M}$  is a diagonal matrix of the wave numbers  $\mu_m$  (12[5]),  $\zeta$  is the Z-transform variable, and the matrix  $\boldsymbol{R}$  has elements

$$r_{lm} = \prod_{j=0}^{l-1} \left(1 + \dot{w}_j s_m\right) / \prod_{j=0}^{l} \left(1 + w_j s_m\right).$$
(5)

The functions  $s_m(\zeta)$  are the roots of the characteristic polynomial

$$\mathcal{P}(s) = \zeta \prod_{l=0}^{L-1} (1+w_l s) - \prod_{l=0}^{L-1} (1+\dot{w}_l s).$$
(6)

The NLBC in the coordinate space is given by the inverse Z transformation of Eq. (4).

#### 3. REFLECTION FROM AN NLBC INTERFACE

Assume there is an NLBC interface between the media one (depth indexes  $j \leq J$ ) and two (depth indexes j > J). Both media are range-independent along the interface. It is also assumed that they are independent of depth within a small stripe along the interface, although this condition is strictly required only for the two depth indexes J and J + 1, one of which is virtual for each of the media. The Z-transformed partial pressure and energy flux fields in the upper medium are combinations of incoming and outgoing plane waves given by Eq. (19[5]):

$$u_{j}^{l} = \rho^{-1/2} \sum_{m=0}^{L-1} \left( B_{m}^{l,+} \mu_{m}^{j-J} + B_{m}^{l,-} \mu_{m}^{J-j} \right), \, \vartheta_{j}^{l} = \sum_{m=0}^{L-1} \left( A_{m}^{l,+} \mu_{m}^{j-J} + A_{m}^{l,-} \mu_{m}^{J-j} \right).$$
(7)

According to Eq. (14[5]), the plane wave amplitudes are related as  $A_m^{l,\pm} = r_{lm}B_m^{0,\pm}$ . Assume that these partial pressure vectors are also related by an NLBC  $\vartheta_{J+1} = T\vartheta_J$ . The particular matrix T is irrelevant for now. Then, one can express  $B^{0,-} = (B_0^{0,-} \dots, B_{L-1}^{0,-})^T$  through  $B^{0,+}$  and T:

$$B^{0,-} = SB^{0,+}$$
, where  $S = [R^{-1}TR - M^{-1}]^{-1}[M - R^{-1}TR]$ . (8)

<sup>&</sup>lt;sup>†</sup>From now on the respective formulas of the referenced literature are denoted as (15[5]).

The matrix S is a reflection matrix expressing the amplitudes of the outgoing waves through the amplitudes of the incoming waves. Similarly to Eq. (8), one can express the NLBC matrix T through the reflection matrix S:

$$T = R(M + M^{-1}S)(E + S)^{-1}R^{-1}.$$
(9)

Note that equations (8) and (9) relate the partial pressures and plane wave amplitudes in the same medium. If the depth nodes J, J+1 are separated by an interface with density discontinuity, one must consider several possible NLBC matrices relating the partial pressure in the upper medium (as above), in two media, and in the lower medium.

Consider now the reflection matrix for the special case when the NLBC is applied at an interface of two homogeneous media. The partial pressures in the lower medium j > J are related by the radiation NLBC (4). The matrix  $\mathbf{R}$  depends only on the PE coefficients, and therefore, is the same for both media. On the contrary, the eigenvalues  $\mu_m$  depend on the sound speed in the medium, so that there are two matrices  $\mathbf{M}_{<}$  and  $\mathbf{M}_{>}$  for the upper and lower media respectively. The NLBC in the upper medium is given by Eq. (18[5]) (the notation > and < is reverted in this paper *cf.* notation in [5]):

$$\boldsymbol{\vartheta}_{J+1,<} = \left[g\boldsymbol{T}_{>} + \boldsymbol{E}\right] \left[\boldsymbol{T}_{>} + g\boldsymbol{E}\right]^{-1} \boldsymbol{\vartheta}_{J,<} = \boldsymbol{T}_{<} \boldsymbol{\vartheta}_{J,<} \,. \tag{10}$$

Here,  $g = g(\tau_{J,<}, \tau_{J,>}) = (\tau_{J,<} + \tau_{J,>})/(\tau_{J,<} - \tau_{J,>})$ , where  $\tau_j = 0.5(\rho_{j+1}^{-1} + \rho_j^{-1})$ , and  $\boldsymbol{E}$  is a unit matrix of size L. Substitution of this expression into Eq. (8) gives

$$\boldsymbol{S} = \left[\boldsymbol{D} - \boldsymbol{M}_{<}^{-1}\right]^{-1} \left[\boldsymbol{M}_{<} - \boldsymbol{D}\right], \text{ where}$$
(11)

$$\boldsymbol{D} \equiv \boldsymbol{R}^{-1} \boldsymbol{T}_{<} \boldsymbol{R} = (g\boldsymbol{M}_{>} + \boldsymbol{E}) (\boldsymbol{M}_{>} + g\boldsymbol{E})^{-1}.$$
 (12)

As all the matrices in the right-hand sides of these equations are diagonal, the matrices D and S are also diagonal. Thus, although the discrete PE has L vertical wavenumbers for each horizontal wavenumber, these waves do not transform one into another at an interface of two media.

#### 4. REFLECTION FROM MULTIPLE LAYERS

Consider now a more general problem when the medium is composed of three layers denoted "1"  $(j \leq J)$ , "2"  $(J < j \leq K)$ , and "3" (j > K). The layers 2 and 3 are homogeneous, while the upper layer 1 is range-independent along the boundary. The amplitudes of plane waves in the three layers are distinguished with an extra subscript such as  $B_{m,1}^{l,\pm}$  for the first layer. It is also assumed that the phases of the plane waves in layers 2 and 3 are counted from the interface at j = K, *i.e.*, the power terms in Eq. (7) have  $\pm (j - K)$  instead of  $\pm (j - J)$ . Under these assumptions, the amplitudes

of incoming and outgoing waves in the layer 2 are related as  $B_2^{0,-} = S_{23}B_2^{0,+}$ , where  $S_{23}$  is the reflection matrix on the interface of layers 2 and 3 given by Eq. (11) with substitution of  $M_3$  for  $M_>$ ,  $M_2$  for  $M_<$ ,  $\tau_3$  for  $\tau_>$ , and  $\tau_2$  for  $\tau_<$ .

The partial pressure fields in the layer 2 near the upper layer boundary are

$$\boldsymbol{\vartheta}_{J,2} = \boldsymbol{R} \big( \boldsymbol{M}_2^{-(K-J)} + \boldsymbol{M}_2^{K-J} \boldsymbol{S}_{23} \big) \boldsymbol{B}_2^{0,+}, \\ \boldsymbol{\vartheta}_{J+1,2} = \boldsymbol{R} \big( \boldsymbol{M}_2^{-(K-J-1)} + \boldsymbol{M}_2^{K-J-1} \boldsymbol{S}_{23} \big) \boldsymbol{B}_2^{0,+},$$
(13)

where  $B_2^{0,-}$  were expressed through  $B_2^{0,+}$ . Excluding  $B_2^{0,+}$  from these equations gives NLBC for the middle layer  $\vartheta_{J+1,2} = T_{2,J}\vartheta_{J,2}$  with the matrix

$$T_{2,J} = R \left[ M_2^{J+1-K} + M_2^{K-J-1} S_{23} \right] \left[ M_2^{J-K} + M_2^{K-J} S_{23} \right]^{-1} R^{-1}.$$
 (14)

The extra index J in  $T_{2,J}$  highlights that the matrix is applied at the upper interface j = J as opposed to the lower interface j = K. Finally, the relationship (10) yields the Z-transformed NLBC for the upper medium

$$\boldsymbol{\vartheta}_{J+1,1} = \boldsymbol{T}_1 \boldsymbol{\vartheta}_{J,1}, \text{ where } \boldsymbol{T}_1 = \left[g_{12}\boldsymbol{T}_{2,J} + \boldsymbol{E}\right] \left[\boldsymbol{T}_{2,J} + g_{12}\boldsymbol{E}\right]^{-1},$$
(15)

with  $g_{12} = g(\tau_1, \tau_2)$ . According to Eq. (8), the reflection matrix at the interface 1–2 is

$$S_{12} = \left[ R^{-1}T_1R - M_1^{-1} \right]^{-1} \left[ M_1 - R^{-1}T_1R \right].$$
(16)

The matrix  $S_{23}$  is diagonal. Hence, the NLBC matrix  $T_{2,J}$  is factored as  $RD_2R^{-1}$ , where the matrix  $D_2$  is also diagonal. Then, the same derivation as in Eq. (12) produces

$$\mathbf{R}^{-1}\mathbf{T}_{1}\mathbf{R} = (g_{12}\mathbf{D}_{2} + \mathbf{E})(\mathbf{D}_{2} + g_{12}\mathbf{E})^{-1}.$$
 (17)

The right-hand side of this expression is diagonal, hence,  $S_{12}$  is diagonal as well. Eq. (17) proves that if the reflection matrix  $S_{23}$  at the lower side of a layer is diagonal, this property is preserved in the reflection matrix  $S_{12}$  at the upper side of this layer.

By induction, Eqs. (14) and (15) allow calculation of the reflection matrices and the Z-transformed NLBC matrices at the upper side of an arbitrary composition of homogeneous liquid layers. Given that the reflection matrices are always diagonal, it is convenient to perform all computations in terms of reflection matrices and then apply Eq. (9) to obtain the Z-transformed NLBC at the final interface.

## 5. NLBC FOR ARBITRARY LAYERED MEDIA

The previous Section 4 presented NLBCs for media consisting of multiple homogeneous layers. Although quite general, this description would require a very large number of layers to approximate real media with continuous variations of their parameters. Moreover, such an approximation may give rise to stability problems due to error accumulation in numerous matrix multiplications. An alternative approach presented in this section is to derive exact discrete NLBC for media with arbitrary variation of the sound speed and density.

Assume that the medium is range-independent below the depth level j = J. The Z-transformed partial pressures in layered media satisfy a system of equations (9[5])

$$u^{l} = \rho^{-1/2} \left[ 1 + w_{l} \hat{\mathbf{X}} \right] \vartheta^{l}, u^{l+1} = \rho^{-1/2} \left[ 1 + \dot{w}_{l} \hat{\mathbf{X}} \right] \vartheta^{l}.$$
(18)

Discretization of  $\hat{\mathbf{X}}$  by Eq. (7[5]) transforms (18) into a system of linear equations

$$u_{j}^{l} = w_{l}A_{j}\vartheta_{j+1}^{l} + (D_{j} + w_{l}B_{j})\vartheta_{j}^{l} + w_{l}C_{j}\vartheta_{j-1}^{l}, \qquad (19a)$$

$$u_{j}^{l+1} = \dot{w}_{l}A_{j}\vartheta_{j+1}^{l} + (D_{j} + \dot{w}_{l}B_{j})\vartheta_{j}^{l} + \dot{w}_{l}C_{j}\vartheta_{j-1}^{l},$$
(19b)

for j = 0, ..., N. The explicit definitions for the arrays  $A_j$ ,  $B_j$ ,  $C_j$ , and  $D_j$  are not significant for this analysis. The source terms are omitted. Dividing Eq. (19a) by  $\dot{w}_l$ , Eq. (19b) by  $w_l$ , and subtracting the results yields

$$u_{j}^{l+1} = u_{j}^{l} \frac{\dot{w}_{l}}{w_{l}} + \left(1 - \frac{\dot{w}_{l}}{w_{l}}\right) \vartheta_{j}^{l} = u_{j}^{0} \mathfrak{P}_{l} + D_{j} \mathfrak{P}_{l} \sum_{k=0}^{l} \frac{1}{\mathfrak{P}_{k}} \left(1 - \frac{\dot{w}_{l}}{w_{l}}\right) \vartheta_{j}^{k}, \qquad (20)$$

where  $\mathfrak{P}_l = \prod_{k=0}^l (\dot{w}_k/w_k)$ . Using the Z transformation shift rule  $u^L = \zeta u^0$  gives

$$u_{j}^{0} = \frac{D_{j}\mathfrak{P}_{L-1}}{\zeta - \mathfrak{P}_{L-1}} \sum_{k=0}^{L-1} \frac{1}{\mathfrak{P}_{k}} \Big( 1 - \frac{\dot{w}_{k}}{w_{k}} \Big) \vartheta_{j}^{k}, \quad u_{j}^{l} = \mathfrak{P}_{l-1} D_{j} \sum_{k=0}^{L-1} \frac{\nu_{lk}}{\mathfrak{P}_{k}} \Big( 1 - \frac{\dot{w}_{k}}{w_{k}} \Big) \vartheta_{j}^{k}, \quad (21)$$

where  $\nu_{lk} = \zeta/(\zeta - \mathfrak{P}_{L-1})$  for k < l and  $\nu_{lk} = \mathfrak{P}_{L-1}/(\zeta - \mathfrak{P}_{L-1})$  for  $k \ge l$ . Substituting Eq. (21) in Eq. (19a) results in a system of equations for the partial pressures

$$w_{l}A_{j}\vartheta_{j+1}^{l} + (D_{j} + w_{l}B_{j})\vartheta_{j}^{l} + w_{l}C_{j}\vartheta_{j-1}^{l} = \mathfrak{P}_{l-1}D_{j}\sum_{k=0}^{L-1}\frac{\nu_{lk}}{\mathfrak{P}_{k}}\Big(1 - \frac{\dot{w}_{k}}{w_{k}}\Big)\vartheta_{j}^{k}.$$
 (22)

The system (22) can be rewritten as Wt = w, where the vector t contains  $\vartheta_j^l$ , j > J, the right-hand side is  $w = -C_{J+1}(w_0\vartheta_J^0, w_1\vartheta_J^1, \dots, w_{L-1}\vartheta_J^{L-1}, 0, \dots)^T$ , and W is a band matrix with 2L + 1 non-zero diagonals. The solution of this linear system is a linear combination of  $\vartheta_J^0, \dots, \vartheta_J^{L-1}$ . Therefore, the partial pressures at the depth node J + 1 are also linear combinations of  $\vartheta_J$ , or, in matrix form,  $\vartheta_{J+1} = T\vartheta_J$ , which is the Z-transformed NLBC for the considered problem. The matrix T is calculated by solving the derived system L times with the right-hand sides  $\vartheta_J^l = \delta_{lk}$ ,  $k = 0, \dots, L - 1$ , and populating the columns of T with  $\vartheta_{J+1}$  obtained for each of the L solutions.

#### 6. DUAL-SIDE NLBC

NLBCs were first proposed for accelerating PE computations by truncating the computational domain [7, 2]. To achieve this benefit, computation of NLBC coefficients must be fast compared to direct PE solution. Alternatively, the coefficients may be precomputed. Looking at the problem from this aspect it is clear that NLBCs provide a form of pre-computation. If propagation conditions in some part of the medium are simple so that a closed-form analytical or semi-analytical solution of the PE is possible, this solution can be cast in the NLBC form so that this part of the medium is excluded from future computations. In this interpretation, NLBCs are not limited to the problems where the environment is simplified at one end of the computational domain. This section presents a practical example of such a generalized NLBC for the simple case of a medium homogeneous between the PE depth nodes J and K. The top and bottom layers may have arbitrary range and depth dependence.

The Z-transformed partial pressure and energy flux fields are given by Eq. (7). It is assumed that there are no density jumps at the interfaces. Hence,  $\vartheta_{j,2} \equiv \vartheta_{j,1} \equiv \vartheta_j$ for j = J, J + 1 (*cf.* Section 4) and  $\vartheta_{j,2} \equiv \vartheta_{j,3} \equiv \vartheta_j$  for j = K, K + 1. Similarly, *cf.* Section 4 the layer sub-index is omitted in the notation for the plane wave amplitudes and the eigenvalue matrix M in the homogeneous middle layer. Expressing the partial pressures  $\vartheta_j$  at the near-interface depth layers j = J, J+1, K, J+1 through the plane wave amplitudes  $B^{0,\pm}$ , then excluding the plane wave amplitudes from the obtained equations and expressing  $\vartheta_{J+1}$  and  $\vartheta_K$  through  $\vartheta_{K+1}$  and  $\vartheta_J$  yields

$$\vartheta_{J+1} = \boldsymbol{R} \boldsymbol{D}_{\text{far}} \boldsymbol{R}^{-1} \vartheta_{K+1} + \boldsymbol{R} \boldsymbol{D}_{\text{near}} \boldsymbol{R}^{-1} \vartheta_{J},$$
  
$$\vartheta_{K} = \boldsymbol{R} \boldsymbol{D}_{\text{near}} \boldsymbol{R}^{-1} \vartheta_{K+1} + \boldsymbol{R} \boldsymbol{D}_{\text{far}} \boldsymbol{R}^{-1} \vartheta_{J},$$
 (23)

with the diagonal matrices  $D_{\text{near}}$  and  $D_{\text{far}}$  defined as

$$\boldsymbol{D}_{\text{near}} = \left[\boldsymbol{M}^{K-J} - \boldsymbol{M}^{J-K}\right] \left[\boldsymbol{M}^{K-J+1} - \boldsymbol{M}^{J-K-1}\right]^{-1},$$
$$\boldsymbol{D}_{\text{far}} = \left[\boldsymbol{M} - \boldsymbol{M}^{-1}\right] \left[\boldsymbol{M}^{K-J+1} - \boldsymbol{M}^{J-K-1}\right]^{-1}.$$
(24)

The system of equations (23) gives the Z-transformed NLBC for the considered problem. After the inverse Z transformation, it represents the partial pressures at the depth nodes J+1 and K as linear combinations of partial pressures at the nodes J and K+1at the current and previous PE steps. Using these expressions, one can split the original L three-diagonal systems of equations into 2L coupled subsystems for  $j \leq J$  and  $j \geq K+1$ . The nodes  $J+1 \leq j \leq K$  can be omitted from computations.

#### 7. SUMMARY

The presented research generalizes the method of NLBCs for arbitrary stratified acoustic media behind the NLBC interface. The NLBC approach provides better accuracy and fewer user-defined parameters as compared to the absorbing "sponge" technique, facilitating automated computations. Calculation of NLBC coefficients for a reasonably complex problem may be comparable in CPU time to the direct solution of the PE in the medium extended by the stratified layers. The performance improvements of the NLBC approach are dramatic when the PE solution is repeated multiple times over the same range-independent part of the medium. Examples include such CPU-heavy tasks as source localization and ocean acoustic tomography through matched-field processing [1], broadband calculations, and Nx2D simulations over azimuth-independent deep bottom. In these applications, NLBC approach becomes a generic pre-computation technique that allows reusing the calculations performed for the range-independent part of the medium, such as the deep water layer or the bottom. Once understood as a variant of pre-computation, the NLBC approach is readily extended to new problems. For example, the dual-side NLBC (23) allows excluding the internal homogeneous strata from the PE calculations.

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