

OPTIMIZING GREEN'S FUNCTIONS IN GROUNDED LAYERED MEDIA WITH ARTIFICIAL BOUNDARY CONDITIONS

L. F. Knockaert

Department Intec-Imec
Ghent University
St. Pietersnieuwstraat 41, B-9000 Gent, Belgium

Abstract—Artificial boundary conditions, which can be identified as Robin boundary conditions positioned at a complex space coordinate, are introduced in order to obtain pertinent approximations for the Green's functions in grounded layered media. These artificial boundary conditions include perfectly matched layers backed by perfectly electric or magnetic conductors. As a first result, we obtain analytical expressions for the differences of Green's functions subject to different boundary conditions. Since weighted sums of Green's functions are again Green's functions, the need arises to solve an optimization problem, in the sense of obtaining the optimal weighted mixture of Green's functions, as compared to the exact Green's function. Comprehensive eigenexpansions for the Green's functions are given in the general case, and a few examples illustrate the goodness of fit between the approximate Green's functions and the exact Green's function.

1. INTRODUCTION

In 1994 Berenger [1] proposed the perfectly matched layer (PML) to truncate computational domains for use in the numerical solution of Maxwell's equations, without introducing reflections. The original split-field approach of Berenger was reformulated in [2] in terms of complex coordinate stretching and in [3] in terms of perfectly matched anisotropic absorbers. More generally it was shown in [4] that the complex coordinate stretching and diagonal anisotropy formulations are equivalent in a general orthogonal coordinate system setting.

Although PML's can be used as absorbing boundary conditions in numerical finite difference [5] and/or finite element techniques, it turns out that they also have applications in semi-analytical techniques. For instance in [6] an approximate eigenmode series expansion for the Green's function of an open layered substrate was obtained by using a PML backed by a perfect electrical conductor (PEC) to turn the originally open layered configuration into an closed waveguiding system. For a more complete bibliography regarding the above approach, together with some pertinent mathematical approximation aspects of the PML method, we refer the reader to [7]. In that paper the PML-PEC combination was identified as a Dirichlet boundary condition positioned at a complex space coordinate or, putting it more bluntly, a layer of complex thickness backed by a PEC plate.

In this paper we consider grounded Green's functions, i.e. Green's functions with a Dirichlet condition at $z = 0$, which can be thought of as the current return ground plane in actual layered circuitry. We treat the general case of artificial boundary conditions (ArBC) which can be identified (but not exhaustively) as Robin boundary conditions positioned at a complex space coordinate. This includes PML-PEC, but also the Neumann ArBC, which consists of a layer of complex thickness backed by a perfectly magnetic conductor (PMC). The goodness of fit of a given ArBC is then determined by the way it compares to the exact outgoing Robin boundary condition (ORBC). It is therefore necessary to obtain expressions for the difference of Green's functions subject to different ArBC's. This is treated in Section 2. Next, since weighted sums of Green's functions are again Green's functions (under certain conditions), the problem of Green's function optimization, in the sense of obtaining the optimal weighted mixture of ArBC Green's functions, is tackled in Section 3. Last but not least, in Section 4, comprehensive eigenexpansions for the Green's functions are given in the ArBC and mixture cases, and a few examples are proposed to illustrate the goodness of fit between the different ArBC or mixture Green's functions and the exact ORBC Green's function.

2. THE GROUNDED HANKEL DOMAIN

Any laterally symmetric scalar Green's function in a layered medium satisfies the source Helmholtz equation [8]

$$\nabla^2 G(\rho, z, z') + \kappa(z)^2 G(\rho, z, z') = \frac{1}{2\pi\rho} \delta(\rho)\delta(z - z') \quad (1)$$

together with appropriate boundary conditions. With radiation conditions [7] in the lateral direction, we can write this in the Hankel

domain as

$$-\gamma^2 \tilde{G}(\gamma, z, z') + \frac{d^2}{dz^2} \tilde{G}(\gamma, z, z') + \kappa(z)^2 \tilde{G}(\gamma, z, z') = \delta(z - z') \quad (2)$$

where $G(\rho, z, z')$ is retrieved by means of the Hankel transform

$$G(\rho, z, z') = \frac{1}{2\pi} \int_0^\infty J_0(\gamma\rho) \tilde{G}(\gamma, z, z') \gamma d\gamma \quad (3)$$

Note also the Bessel-Parseval relation [9]

$$\int_0^\infty |G(\rho, z, z')|^2 2\pi\rho d\rho = \frac{1}{2\pi} \int_0^\infty |\tilde{G}(\gamma, z, z')|^2 \gamma d\gamma \quad (4)$$

Applying different boundary conditions to (2) will lead to different solutions in the Hankel domain.

For example the Green's function for a uniform halfspace ($\kappa(z) = k_0$, where $k_0 = \omega/c$ is the free-space wavenumber, assuming a $e^{i\omega t}$ time dependence) grounded at $z = 0$ is analytically given by

$$G_H(\rho, z, z') = \frac{e^{-ik_0\sqrt{\rho^2+(z+z')^2}}}{4\pi\sqrt{\rho^2+(z+z')^2}} - \frac{e^{-ik_0\sqrt{\rho^2+(z-z')^2}}}{4\pi\sqrt{\rho^2+(z-z')^2}} \quad (5)$$

which transforms in the Hankel domain to [10]

$$\tilde{G}_H(\gamma, z, z') = -\frac{1}{\beta} \sin \beta z_{<} e^{-i\beta z_{>}} \quad (6)$$

where

$$\beta = \sqrt{k_0^2 - \gamma^2} \quad z_{<} = \min(z, z') \quad z_{>} = \max(z, z') \quad (7)$$

Note that β belongs to the branch cut line Γ formed by the negative imaginary axis \mathbf{I}_- and the real interval $[0, k_0] \subset \mathbf{R}_+$. Now let the region of interest be $0 \leq z, z' \leq 1$, such that there is a certain amount of free space left, i.e., $\kappa(z) = k_0$ for $z \in [1 - \iota, 1]$, where $0 < \iota \leq 1$. We can write equation (2) with the new parameter β as

$$\beta^2 \tilde{G}(\beta, z, z') + \frac{d^2}{dz^2} \tilde{G}(\beta, z, z') - U(z) \tilde{G}(\beta, z, z') = \delta(z - z') \quad (8)$$

where

$$U(z) = k_0^2 - \kappa(z)^2 \quad (9)$$

Besides the grounded Dirichlet condition $\tilde{G}(\beta, 0, z') = 0$ we must also fix a boundary condition at $z = 1$. To obtain outgoing waves at $z = 1$ we need, in accordance with (6), the ORBC

$$\tilde{G}'(\beta, 1, z') = -i\beta\tilde{G}(\beta, 1, z') \quad (10)$$

The problem with the ORBC is that it depends on β and hence on the Hankel transform variable γ . We would be more pleased with a Robin boundary condition (RBC)

$$\tilde{G}'(\beta, 1, z') = \tau\tilde{G}(\beta, 1, z') \quad (11)$$

with τ a constant, since an expansion in terms of the eigenfunctions and eigenvalues of the differential operator

$$\mathcal{L}y = \frac{d^2}{dz^2}y(z) + \kappa(z)^2y(z) \quad (12)$$

with boundary conditions $y(0) = 0$ and $y'(1) = \tau y(1)$, see Section 4, would then offer an elegant pathway to an eigendecomposition of the Green's function. Note that $\tau = 0$ corresponds with Neumann boundary conditions and $\tau = \infty$ with Dirichlet boundary conditions. Unfortunately, as $\tau \neq -i\beta$, the Green's function thus obtained would certainly be not sufficiently close to the Green's function with ORBC. Another, more promising approach is the ArBC method. Suppose that the Green's function can be extended such that z belongs to \mathcal{C} . Then we could impose a constant parameter RBC at $z = b$, where $b \in \mathcal{C}$. In other words we require

$$\tilde{G}'(\beta, b, z') = \tau\tilde{G}(\beta, b, z') \quad (13)$$

Now of course, when imposing the ArBC (13) leads to a unique grounded Green's function, this will in general trace back to a non-constant RBC at $z = 1$, namely

$$\tilde{G}'(\beta, 1, z') = \eta_\tau(\beta)\tilde{G}(\beta, 1, z') \quad (14)$$

In the event we were lucky enough to find $\eta_\tau(\beta) = -i\beta$, this would of course solve the problem. If this is not the case, then it is important to compare the Green's functions with ORBC and RBC defined by $\eta_\tau(\beta)$, respectively. In general we have the following

Theorem: Let $\tilde{G}_{1,2}(\beta, z, z')$ be two Green's functions satisfying equation (8) with Dirichlet condition at $z = 0$ and respective non-constant RBC's

$$\tilde{G}'_{1,2}(\beta, 1, z') = \eta_{1,2}(\beta)\tilde{G}_{1,2}(\beta, 1, z') \quad (15)$$

at $z = 1$. Then the error function $\tilde{E}(\beta, z, z') = \tilde{G}_1(\beta, z, z') - \tilde{G}_2(\beta, z, z')$ can be written as

$$\tilde{E}(\beta, z, z') = \frac{\phi(\beta, z)\phi(\beta, z')}{\phi(\beta, 1)^2} \left[\frac{1}{\eta_1(\beta) - \phi'(\beta, 1)/\phi(\beta, 1)} - \frac{1}{\eta_2(\beta) - \phi'(\beta, 1)/\phi(\beta, 1)} \right] \quad (16)$$

where the regular solution $\phi(\beta, z)$ satisfies the homogeneous equation

$$\beta^2 \phi(\beta, z) + \frac{d^2}{dz^2} \phi(\beta, z) - U(z)\phi(\beta, z) = 0 \quad (17)$$

with boundary conditions $\phi(\beta, 0) = 0$, $\phi'(\beta, 0) = 1$.

Proof : The Green's function $\tilde{G}_1(\beta, z, z')$ can be written as

$$\tilde{G}_1(\beta, z, z') = -\phi(\beta, z_{<}) \frac{\xi_1(\beta, z_{>})}{\xi_1(\beta, 0)} \quad (18)$$

where $\xi_1(\beta, z)$ is another independent solution of (17) satisfying the RBC

$$\xi_1'(\beta, 1) = \eta_1(\beta)\xi_1(\beta, 1) \quad (19)$$

Since $\xi_1(\beta, z)$ can be written as

$$\xi_1(\beta, z) = A_1(\beta)\phi(\beta, z) + \phi(\beta, z) \int_z^1 \frac{ds}{\phi(\beta, s)^2} \quad (20)$$

where $A_1(\beta)$ is determined by the RBC as

$$A_1(\beta)\phi'(\beta, 1) - \frac{1}{\phi(\beta, 1)} = A_1(\beta)\eta_1(\beta)\phi(\beta, 1) \quad (21)$$

and since

$$\xi_1(\beta, 0) = \lim_{z \rightarrow 0} \phi(\beta, z) \int_z^1 \frac{ds}{\phi(\beta, s)^2} = 1 \quad (22)$$

by de L'Hospital's rule, we simply find that

$$\tilde{G}_1(\beta, z, z') = -\phi(\beta, z_{<})\xi_1(\beta, z_{>}) \quad (23)$$

Hence we have that the difference between the two Green's functions is

$$\begin{aligned} \tilde{G}_1(\beta, z, z') - \tilde{G}_2(\beta, z, z') &= -\phi(\beta, z_{<})(\xi_1(\beta, z_{>}) - \xi_2(\beta, z_{>})) \\ &= -\phi(\beta, z)\phi(\beta, z')(A_1(\beta) - A_2(\beta)) \end{aligned} \quad (24)$$

which can be written as (16). \square

Corollary : Let $\tilde{G}_1(\beta, z, z')$ satisfy the ORBC (10) and $\tilde{G}_2(\beta, z, z')$ satisfy the ArBC (13). Then the error function $\tilde{E}(\beta, z, z') = \tilde{G}_1(\beta, z, z') - \tilde{G}_2(\beta, z, z')$ can be written as

$$\begin{aligned} \tilde{E}(\beta, z, z') = & -\phi(\beta, z)\phi(\beta, z') \left[\frac{1}{\phi(\beta, 1)(\phi'(\beta, 1) + i\beta\phi(\beta, 1))} \right. \\ & \left. - \frac{1}{\phi(\beta, b)(\phi'(\beta, b) - \tau\phi(\beta, b))} - \int_1^b \frac{dz}{\phi(\beta, z)^2} \right] \end{aligned} \quad (25)$$

Proof : Since $\tilde{G}_2(\beta, z, z')$ satisfies (13) at $z = b$, we can write it as

$$\tilde{G}_2(\beta, z, z') = -\phi(\beta, z_{<}) \frac{\xi(\beta, z_{>})}{\xi(\beta, 0)} \quad (26)$$

where $\tau = \xi'(\beta, b)/\xi(\beta, b)$. Now $\xi(\beta, z)$ can be written as

$$\xi(\beta, z) = A(\beta)\phi(\beta, z) + \phi(\beta, z) \int_z^b \frac{ds}{\phi(\beta, s)^2} \quad (27)$$

where $A(\beta)$ is determined by the ArBC as

$$A(\beta)\phi'(\beta, b) - \frac{1}{\phi(\beta, b)} = \tau A(\beta)\phi(\beta, b) \quad (28)$$

Traced back to $z = 1$ we obtain that

$$\eta_2(\beta) = \frac{\phi'(\beta, 1)}{\phi(\beta, 1)} - \frac{1}{\phi(\beta, 1)^2 \left(A(\beta) + \int_1^b \frac{dz}{\phi(\beta, z)^2} \right)} \quad (29)$$

Solving (28) for $A(\beta)$ and inserting $\eta_2(\beta)$ and $\eta_1(\beta) = -i\beta$ in (16) we obtain (25). \square

Now since $U(z) \equiv 0$ for $z \geq 1$, the regular solution $\phi(\beta, z)$ can be analytically continued in $z > 1$ and in fact for $\Re z > 1$. This means that the values of the regular solution and its derivative at $z = b$, with $\Re b > 1$, can be traced back to the values at $z = 1$ by means of

$$\phi(\beta, b) = \phi'(\beta, 1) \frac{\sin \beta(b-1)}{\beta} + \phi(\beta, 1) \cos \beta(b-1) \quad (30)$$

$$\phi'(\beta, b) = \phi'(\beta, 1) \cos \beta(b-1) - \beta\phi(\beta, 1) \sin \beta(b-1) \quad (31)$$

Similarly we have that

$$\int_1^b \frac{dz}{\phi(\beta, z)^2} = \frac{\sin \beta(b-1)}{\beta \phi(\beta, 1) \phi(\beta, b)} = \frac{1}{\phi(\beta, 1) (\phi'(\beta, 1) + \beta \phi(\beta, 1) \cot \beta(b-1))} \quad (32)$$

It is seen that inserting (30)–(32) in (25) leads to an expression solely depending on $\phi(\beta, z)$ and its derivative with values inside $[0, 1]$ and other functions depending on β, b . In the important Dirichlet case $\tau = \infty$ expression (25) becomes

$$\tilde{E}_D(\beta, z, z') = -\frac{\phi(\beta, z)\phi(\beta, z')}{\phi(\beta, 1)} \left[\frac{1}{\phi'(\beta, 1) + i\beta\phi(\beta, 1)} - \frac{1}{\phi'(\beta, 1) + \beta\phi(\beta, 1) \cot \beta(b-1)} \right] \quad (33)$$

and in the equally important Neumann case $\tau = 0$ we obtain

$$\tilde{E}_N(\beta, z, z') = -\frac{\phi(\beta, z)\phi(\beta, z')}{\phi(\beta, 1)} \left[\frac{1}{\phi'(\beta, 1) + i\beta\phi(\beta, 1)} - \frac{1}{\phi'(\beta, 1) - \beta\phi(\beta, 1) \tan \beta(b-1)} \right] \quad (34)$$

It should be noted that, except for the Robin parameter τ and the complex thickness b , the difference between the Green's functions in (25), (33) and (34) is completely determined by the regular solution $\phi(\beta, z)$. For $U(z) \equiv 0$ the regular solution is readily obtained as $\phi(\beta, z) = \sin(\beta z)/\beta$, whereas for $U(z) \neq 0$, the regular solution satisfies the Volterra integral equation

$$\phi(\beta, z) = \frac{\sin \beta z}{\beta} + \int_0^z \frac{\sin[\beta(z-z')]}{\beta} U(z')\phi(\beta, z') dz' \quad (35)$$

The derivative $\phi'(\beta, z)$ is recovered by means of

$$\phi'(\beta, z) = \cos \beta z + \int_0^z \cos[\beta(z-z')] U(z')\phi(\beta, z') dz' \quad (36)$$

It is known [11] that

$$|\phi(\beta, z)| \leq \frac{\exp(|\Im \beta|z)}{|\beta|} \exp \left[\frac{1}{|\beta|} \int_0^z |U(z')| dz' \right] \quad (37)$$

when $\beta \neq 0$. A better bound, valid for all $\beta \in \mathbf{C}$, was obtained in [12]:

$$|\phi(\beta, z)| \leq \exp(|\Im\beta|z) \frac{Cz}{1+z|\beta|} \exp \left[C \int_0^z |U(z')| \frac{z'}{1+z'|\beta|} dz' \right] \quad (38)$$

and a slightly weaker bound is found in [13]:

$$|\phi(\beta, z)| \leq \exp(|\Im\beta|z) \frac{Cz}{1+z|\beta|} \exp \left[Cz \int_0^z |U(z')| dz' \right] \quad (39)$$

The universal constant C in (38)–(39) is given by

$$C = \sup_{z \in \mathbf{C}} \frac{|\sin(z)|(1+|z|)}{|z| \exp(|\Im z|)} \quad (40)$$

Expressions (37)–(39) define $\phi(\beta, z)$ as an entire function in the whole β -plane for all fixed $0 < z \leq 1$, provided $\int_0^1 |U(z)| dz < \infty$. It should be noted [11, 12] that $\phi(\beta, z) \rightarrow \sin(\beta z)/\beta$ when $z \rightarrow 0$ and also when $|\beta| \rightarrow \infty$. Lastly, from bound (39), one can easily infer [13] that $\phi(\beta, z)$, for fixed $0 < z \leq 1$, belongs to the class of Paley-Wiener entire functions [14] \mathbf{B}_z^p , $p > 1$. This implies that for all $0 < z \leq 1$ and for all $\beta \in \mathbf{C}$ we can write down the cardinal series

$$\phi(\beta, z) = \sum_{n \in \mathbf{Z}} \phi \left(\frac{n\pi}{z}, z \right) \operatorname{sinc}(\beta z - n\pi) \quad (41)$$

and, see (36) and [13]:

$$\phi'(\beta, z) = \cos \beta z + \sum_{n \in \mathbf{Z}} \left[\phi' \left(\frac{n\pi}{z}, z \right) - (-1)^n \right] \operatorname{sinc}(\beta z - n\pi) \quad (42)$$

3. OPTIMIZING GREEN'S FUNCTIONS

Let $\tilde{G}_0(\beta, z, z')$ be the exact Green's function with ORBC in the Hankel domain. Then the Green's function in the spatial domain can be found by means of the Hankel transform

$$G_0(\rho, z, z') = \frac{1}{2\pi} \int_0^\infty J_0(\gamma\rho) \tilde{G}_0 \left(\sqrt{k_0^2 - \gamma^2}, z, z' \right) \gamma d\gamma \quad (43)$$

This would be the end of the story, were it not for the fact that the Hankel transform a.k.a. Sommerfeld integral (43) is notoriously hard to evaluate [7], because the integrand is often highly oscillatory and exhibits singularities of the pole *and* branchpoint type. Hence our

purpose is to avoid the Sommerfeld integral approach altogether and to approximate $\tilde{G}_0(\beta, z, z')$ in the Hankel domain by a mixture of Green's functions of the ArBC type for which, as will be shown in Section 4, explicit eigenexpansions can be written down. Hence we propose the approximation

$$\tilde{G}_0(\beta, z, z') \approx \sum_{k=1}^M q_k \tilde{G}_k(\beta, z, z') \quad (44)$$

where, for this approximation to be a valid Green's function, we must require that the complex coefficients q_k are such that

$$\sum_{k=1}^M q_k = 1 \quad (45)$$

The overall error $\tilde{E}(\beta, z, z')$ can be written as

$$\tilde{E}(\beta, z, z') = \tilde{G}_0(\beta, z, z') - \sum_{k=1}^M q_k \tilde{G}_k(\beta, z, z') = \sum_{k=1}^M q_k \tilde{E}_k(\beta, z, z') \quad (46)$$

where $\tilde{E}_k(\beta, z, z') = \tilde{G}_0(\beta, z, z') - \tilde{G}_k(\beta, z, z')$. From the Bessel-Parseval relation (4) we infer that minimizing the weighted squared error

$$\mathcal{E} = \frac{1}{2\pi} \int_0^\infty |\tilde{E}(\beta, z, z')|^2 \gamma d\gamma \quad (47)$$

in the Hankel domain is equivalent with minimizing the same weighted squared error in the spatial domain.

There remains to find particular choices for z, z' . From the Corollary and since the bounds (37)–(39) are strictly increasing with z , it seems natural to take $z = z' = 1$, the endpoint of the interval under consideration. Since $\beta d\beta = -\gamma d\gamma$, we can redefine the weighted squared error \mathcal{E} as

$$\mathcal{E} = \frac{1}{2\pi} \int_0^{k_0} |\tilde{E}(\beta, 1, 1)|^2 \beta d\beta + \frac{1}{2\pi} \int_0^\infty |\tilde{E}(-i\beta, 1, 1)|^2 \beta d\beta \quad (48)$$

Defining the Grammian matrix K as

$$\begin{aligned} K_{k,l} &= \frac{1}{2\pi} \int_0^{k_0} \overline{\tilde{E}_k(\beta, 1, 1)} \tilde{E}_l(\beta, 1, 1) \beta d\beta \\ &+ \frac{1}{2\pi} \int_0^\infty \overline{\tilde{E}_k(-i\beta, 1, 1)} \tilde{E}_l(-i\beta, 1, 1) \beta d\beta \end{aligned} \quad (49)$$

it is straightforward to show that the solution of the constrained minimization of \mathcal{E} under constraint (45) is given by the vector

$$q = K^{-1}f/f^*K^{-1}f \quad (50)$$

where f is a vector with all its entries ones. The minimum value for \mathcal{E} is given by

$$\mathcal{E} = q^*Kq = 1/f^*K^{-1}f \quad (51)$$

By construction, we have that the minimal value satisfies $\mathcal{E} \leq \min_k K_{k,k}$, and hence, in order to measure the amelioration produced by the optimization procedure, we can define the enhancement factor \mathcal{A} as

$$\mathcal{A} = \min_k K_{k,k}/\mathcal{E} \geq 1 \quad (52)$$

Of course, the integrals (49) defining the entries of the Hermitian symmetric positive definite Grammian matrix K have to be evaluated, and this may be a difficult task. But it is an even more stringent requirement to ensure that these integrals are actually finite. It is sufficient to prove that the diagonal elements $K_{k,k} < \infty$, since by the Cauchy-Schwartz inequality we have that

$$|K_{k,l}|^2 \leq K_{k,k}K_{l,l} \quad (53)$$

If we restrict ourselves to Dirichlet and Neumann ArBC's we have

$$\tilde{E}_D(\beta, 1, 1, b) = \frac{\phi(\beta, 1)}{\phi'(\beta, 1) + \beta\phi(\beta, 1)\cot\beta(b-1)} - \frac{\phi(\beta, 1)}{\phi'(\beta, 1) + i\beta\phi(\beta, 1)} \quad (54)$$

and

$$\tilde{E}_N(\beta, 1, 1, b) = \frac{\phi(\beta, 1)}{\phi'(\beta, 1) - \beta\phi(\beta, 1)\tan\beta(b-1)} - \frac{\phi(\beta, 1)}{\phi'(\beta, 1) + i\beta\phi(\beta, 1)} \quad (55)$$

Since $\phi(\beta, z)$ and $\phi'(\beta, z)$ tend to the unperturbed functions $\sin(\beta z)/\beta$ and $\cos(\beta z)$, respectively, for $|\beta| \rightarrow \infty$ [12], we can insert these unperturbed functions in (54) and (55), yielding

$$\tilde{E}_{D,\infty}(\beta, 1, 1, b) = 2i \frac{\sin^2\beta}{\beta(1 - e^{2i\beta b})} \quad (56)$$

and

$$\tilde{E}_{N,\infty}(\beta, 1, 1, b) = 2i \frac{\sin^2 \beta}{\beta (1 + e^{2i\beta b})} \quad (57)$$

For integrals of the form (48) to be finite for $\tilde{E}_{D,\infty}(\beta, 1, 1)$ and $\tilde{E}_{N,\infty}(\beta, 1, 1)$ it is not hard to show by inspection that the complex thickness b must mandatorily belong to the quadrant \mathbf{D}_0 defined as

$$\mathbf{D}_0 = \{z \in \mathbf{C} : \Re z > 1 \quad \text{and} \quad \Im z \leq 0\} \quad (58)$$

However, it is better to work in the open quadrant $\mathbf{D} \subset \mathbf{D}_0$ defined as

$$\mathbf{D} = \{z \in \mathbf{C} : \Re z > 1 \quad \text{and} \quad \Im z < 0\} \quad (59)$$

since when $b \in \mathbf{D}$, it is seen that the error functions $\tilde{E}_{D,\infty}(\beta, 1, 1)$ and $\tilde{E}_{N,\infty}(\beta, 1, 1)$ decrease exponentially when $\beta \rightarrow \infty$ in \mathbf{R}_+ and also when $\beta \rightarrow -i\infty$ in \mathbf{I}_- .

3.1. Examples

As a first example we consider the approximation of the grounded unperturbed halfspace Green's function (5) in the Hankel domain by means of a mixture of $M = 2$ ArBC Green's functions. We take $k_0 = 1$, $b_1 = 1.3 - 0.5i$ and $b_2 = 1.3 - 0.6i$ inside \mathbf{D} . Note of course that $q_2 = 1 - q_1$. For a mixture of two Dirichlet ArBC Green's functions with error functions $\tilde{E}_1(\beta, 1, 1) = \tilde{E}_{D,\infty}(\beta, 1, 1, b_1)$ and $\tilde{E}_2(\beta, 1, 1) = \tilde{E}_{D,\infty}(\beta, 1, 1, b_2)$ we obtain $q_1 = -1.41351 - 3.565961i$ with an enhancement factor $\mathcal{A} = 1.989$. For a mixture of a Dirichlet and a Neumann ArBC Green's functions with error functions $\tilde{E}_1(\beta, 1, 1) = \tilde{E}_{D,\infty}(\beta, 1, 1, b_1)$ and $\tilde{E}_2(\beta, 1, 1) = \tilde{E}_{N,\infty}(\beta, 1, 1, b_1)$ we obtain $q_1 = 0.502025 + 0.112657i$ with a better enhancement factor $\mathcal{A} = 8.82408$. As a second example we consider the one-layer configuration

$$U(z) = u \quad \text{for} \quad 0 \leq z \leq a \leq 1 \quad \text{else} \quad U(z) = 0 \quad (60)$$

The regular solution and its derivative are given by

$$\phi(\beta, z) = \frac{\sin(z\sqrt{\beta^2 - u})}{\sqrt{\beta^2 - u}} \quad \phi'(\beta, z) = \cos(z\sqrt{\beta^2 - u}) \quad (61)$$

for $0 \leq z \leq a$ and (in convenient matrix format)

$$\begin{pmatrix} \phi(\beta, z) \\ \phi'(\beta, z) \end{pmatrix} = \begin{pmatrix} \frac{\sin \beta z}{\beta} & \cos \beta z \\ \cos \beta z & -\beta \sin \beta z \end{pmatrix} \begin{pmatrix} \frac{\sin \beta a}{\beta} & \cos \beta a \\ \cos \beta a & -\beta \sin \beta a \end{pmatrix}^{-1} \cdot \begin{pmatrix} \frac{\sin(a\sqrt{\beta^2 - u})}{\sqrt{\beta^2 - u}} \\ \cos(a\sqrt{\beta^2 - u}) \end{pmatrix} \quad (62)$$

for $a \leq z \leq 1$. The complex thicknesses b_1 and b_2 remain as before and we take $a = 0.5$ and $u = 1$. For a mixture of two Dirichlet ArBC Green's functions with error functions $\tilde{E}_1(\beta, 1, 1) = \tilde{E}_D(\beta, 1, 1, b_1)$ and $\tilde{E}_2(\beta, 1, 1) = \tilde{E}_D(\beta, 1, 1, b_2)$ we obtain $q_1 = -1.3422 - 3.52712i$ with an enhancement factor $\mathcal{A} = 2.01611$. For a mixture of a Dirichlet and a Neumann ArBC Green's functions with error functions $\tilde{E}_1(\beta, 1, 1) = \tilde{E}_D(\beta, 1, 1, b_1)$ and $\tilde{E}_2(\beta, 1, 1) = \tilde{E}_N(\beta, 1, 1, b_1)$ we obtain $q_1 = 0.492679 + 0.110289i$ with a better enhancement factor $\mathcal{A} = 8.69621$. The integrations were performed with the standard MATHEMATICA® function NIntegrate. We may therefore conclude that mixtures of Dirichlet and Neumann ArBC's generally exhibit better enhancement factors.

4. EIGENEXPANSIONS

Suppose we impose the ArBC

$$\tilde{G}'(\beta, b, z') = \tau \tilde{G}(\beta, b, z') \quad (63)$$

with $b \in \mathbf{D}$. Then, taking into account the grounded condition $\tilde{G}(\beta, 0, z') = 0$, it is clear [7, 8] that solving the eigenvalue problem

$$\frac{d^2}{dz^2} \psi(z) + \kappa(z)^2 \psi(z) = -\lambda \psi(z) \quad (64)$$

with boundary conditions

$$\psi(0) = 0, \quad \psi'(b) = \tau \psi(b) \quad (65)$$

leads to a comprehensive series expansion for the spatial Green's function $G(\rho, z, z')$ with defining equation (1), which can be reformulated as

$$\nabla_\rho^2 G(\rho, z, z') + \frac{d^2}{dz^2} G(\rho, z, z') + \kappa(z)^2 G(\rho, z, z') = \frac{1}{2\pi\rho} \delta(\rho) \delta(z - z') \quad (66)$$

Using separation of variables [8] we obtain the Green's function series expansion

$$G(\rho, z, z') = \frac{i}{4} \sum_{n=1}^{\infty} H_0^{(2)}(-i\rho\sqrt{\lambda_n})\psi_n(z)\psi_n(z') \quad (67)$$

where the $\{\psi_n(z)\}$ are the normalized eigenfunctions. From the construction of the regular solution $\phi(\beta, z)$, it is readily verified that the eigenfunctions can be written as

$$\psi_n(z) = d_n\phi(\beta_n, z) \quad (68)$$

and are b -orthonormal in the assumption of non-degeneracy, i.e.,

$$\int_0^b \psi_n(z)\psi_m(z) dz = \delta_{n,m} \quad (69)$$

Note that the complex integration path $[0, b]$ in (69) must consist of the real interval $[0, 1]$ together with a simple Jordan arc from 1 to b . The parameters β_n are obtained by solving the transcendental equation

$$\phi'(\beta, b) = \tau\phi(\beta, b) \quad (70)$$

and the eigenvalues λ_n are given by

$$\lambda_n = \beta_n^2 - k_0^2 \quad (71)$$

Equation (70) can be solved by tracing back to $b = 1$ by means of equations (30)–(31). Furthermore, since the values of $\phi(\beta, 1)$ and $\phi'(\beta, 1)$ for all $\beta \in \mathbf{C}$ are uniquely determined by the values $\phi(n\pi, 1)$ and $\phi'(n\pi, 1)$ with $n \in \mathbf{Z}$, we could utilize the cardinal series (41) and (42) to actually calculate the β_n as in [13]. However, both that approach and the explicit solving of (70) require accurate root finding programs, and these are not in general easily come by. A more appealing technique is the following perturbation approach. Suppose we have obtained the eigenfunctions $\{\chi_n(z)\}$ and the eigenvalues $\{\mu_n\}$ pertaining to the unperturbed eigenvalue problem

$$\frac{d^2}{dz^2} \chi(z) = -\mu\chi(z) \quad (72)$$

with the same boundary conditions

$$\chi(0) = 0, \quad \chi'(b) = \tau\chi(b) \quad (73)$$

If we suppose the $\{\chi_n(z)\}$ complete in $L_2[0, 1]$, we can expand any eigenfunction $\psi_n(z)$ of the original eigenvalue problem (64)–(65) as

$$\psi_n(z) = \sum_k D_{n,k} \chi_k(z) \quad (74)$$

Inserting this in (64) we obtain

$$-\sum_k D_{n,k} \mu_k \chi_k(z) + \kappa(z)^2 \sum_k D_{n,k} \chi_k(z) = -\lambda_n \sum_k D_{n,k} \chi_k(z) \quad (75)$$

Utilizing the b -orthonormality (69) we obtain via Galerkin projection

$$-D_{n,m} \mu_m + \sum_k D_{n,k} \int_0^b \chi_m(z) \kappa(z)^2 \chi_k(z) dz = -\lambda_n D_{n,m} \quad (76)$$

If we truncate the expansions (67) and (74) to their first N terms, the equations (76) can be written in matrix format as

$$D\Upsilon + DP = \Lambda D \quad (77)$$

where the entries of the matrix P are given by

$$P_{k,l} = -\int_0^b \chi_k(z) \kappa(z)^2 \chi_l(z) dz = \int_0^1 \chi_k(z) U(z) \chi_l(z) dz - k_0^2 \delta_{k,l} \quad (78)$$

and $\Upsilon = \text{diag}(\mu_1, \dots, \mu_N)$, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_N)$. The eigendecomposition

$$P + \Upsilon = Q\Lambda Q^{-1} \quad (79)$$

then provides the eigenvalues λ_n and the matrix $D = Q^{-1}$, assuming P diagonalizable. Since P is complex symmetric, in other words $P = P^T$ (but not Hermitian symmetric: $P \neq P^*$ in general), the eigenvectors can be chosen to be complex orthonormal [16], i.e., $Q^T Q = I$, in conformity with the b -orthonormality requirement $DD^T = I$, see (69). Next we discuss the important Dirichlet and Neumann cases.

4.1. The Dirichlet Case

In the unperturbed Dirichlet case $\tau = \infty$, $U(z) = 0$ we have the Hankel domain Green's function

$$\tilde{G}_{D,\infty}(\beta, z, z', b) = -\frac{\sin \beta z_{<}}{\beta} \frac{\sin \beta(b - z_{>})}{\sin \beta b} \quad (80)$$

The corresponding spatial Green's function, being the Hankel transform (3) of (80), can be written [15] as

$$G_{D,\infty}(\rho, z, z', b) = -\frac{1}{4\pi} \int_{\mathbf{R}} H_0^{(2)}(\gamma\rho) \frac{\sin \beta z_{<}}{\beta} \frac{\sin \beta(b - z_{>})}{\sin \beta b} \gamma d\gamma \quad (81)$$

where $\int_{\mathbf{R}}$ stands for an integral over a path in the open lower halfplane just below the branch-cut $[-\infty, 0]$, together with the positive real axis $(0, \infty]$. Since the integrand in (81) is meromorphic in the open lower halfplane, and since $\gamma d\gamma = -\beta d\beta$, we can utilize the residue theorem to write down the expansion

$$G(\rho, z, z') = \frac{i}{4} \sum_{n=1}^{\infty} H_0^{(2)}\left(-i\rho\sqrt{\mu_n - k_0^2}\right) \chi_n(z)\chi_n(z') \quad (82)$$

where the eigensystem $\{\chi_n(z), \mu_n\}$ is given by

$$\chi_n(z) = \sqrt{\frac{2}{b}} \sin\left(\frac{n\pi z}{b}\right) \quad \mu_n = \left(\frac{n\pi}{b}\right)^2 \quad (83)$$

One deduces straightforwardly that the series (82) converges exponentially when

$$\rho > (z + z') \frac{|\Im b|}{\Re b} \quad (84)$$

and diverges exponentially when

$$\rho < (z + z') \frac{|\Im b|}{\Re b} \quad (85)$$

a result which is in conformity with the analysis in [7]. In [10] it was proved that $\{\chi_n(z)\}$ is complete in $L_2[0, 1]$ provided $|b| \geq 1$. The matrix P is given by

$$P_{k,l} = \frac{2}{b} \int_0^1 \sin\left(\frac{k\pi z}{b}\right) U(z) \sin\left(\frac{l\pi z}{b}\right) dz - k_0^2 \delta_{k,l} \quad (86)$$

which can be easily calculated analytically when $U(z)$ is piecewise polynomial, piecewise exponential, etc.

4.2. The Neumann Case

In the unperturbed Neumann case $\tau = 0$, $U(z) = 0$ we have the Hankel domain Green's function

$$\tilde{G}_{N,\infty}(\beta, z, z', b) = -\frac{\sin \beta z_{<}}{\beta} \frac{\cos \beta(b - z_{>})}{\cos \beta b} \quad (87)$$

The corresponding spatial Green's function is given by

$$G_{N,\infty}(\rho, z, z', b) = -\frac{1}{4\pi} \int_{\mathbf{R}} H_0^{(2)}(\gamma\rho) \frac{\sin \beta z_{<} \cos \beta(b - z_{>})}{\beta \cos \beta b} \gamma d\gamma \quad (88)$$

yielding the expansion (82) where the eigensystem $\{\chi_n(z), \mu_n\}$ is now given by

$$\chi_n(z) = \sqrt{\frac{2}{b}} \sin\left(\frac{(n-1/2)\pi z}{b}\right) \quad \mu_n = \left(\frac{(n-1/2)\pi}{b}\right)^2 \quad (89)$$

The series (82) with the Neumann eigensystem (89) converges or diverges under the same conditions as in the Dirichlet case. The matrix P is given by

$$P_{k,l} = \frac{2}{b} \int_0^1 \sin\left(\frac{(k-1/2)\pi z}{b}\right) U(z) \sin\left(\frac{(l-1/2)\pi z}{b}\right) dz - k_0^2 \delta_{k,l} \quad (90)$$

4.3. Examples

We consider the examples treated in Subsection 3.1. Since mixtures of the Neumann and Dirichlet ArBC type exhibit the best enhancement factors we only consider this mixture type ArBC. We take $k_0 = 1$ and the complex thickness $b = 1.3 - 0.5i$. The first example considers the approximation of the grounded unperturbed halfspace Green's function (5) by means of a Neumann-Dirichlet ArBC mixture with $q_1 = 0.502025 + 0.112657i$ and truncation at $N = 32$. The results are shown in Figure 1. It is seen that the mixture ArBC is better than the Neumann or Dirichlet ArBC's taken separately.

The second example considers the one-layer configuration of Subsection 3.1 with $a = 1/2$ and $u = 1$. At the interface $z = z' = a = 1/2$ the ORBC Hankel domain Green's function is

$$\tilde{G}(\gamma, 1/2, 1/2) = \begin{cases} -\frac{1}{i\sqrt{1-\gamma^2} + \gamma \coth(\gamma/2)} & \text{for } 0 \leq \gamma \leq 1 \\ -\frac{1}{\sqrt{\gamma^2-1} + \gamma \coth(\gamma/2)} & \text{for } \gamma \geq 1 \end{cases} \quad (91)$$

The spatial Green's function $G(\rho, 1/2/1/2)$ is obtained via the Hankel transform (3) of (91). We approximate $G(\rho, 1/2/1/2)$ by means of a Neumann-Dirichlet ArBC mixture with $q_1 = 0.492679 + 0.110289i$ and truncation at $N = 32$. Since the imaginary part of $G(\rho, 1/2/1/2)$, in contradistinction with its real part, is easily evaluated by means of a

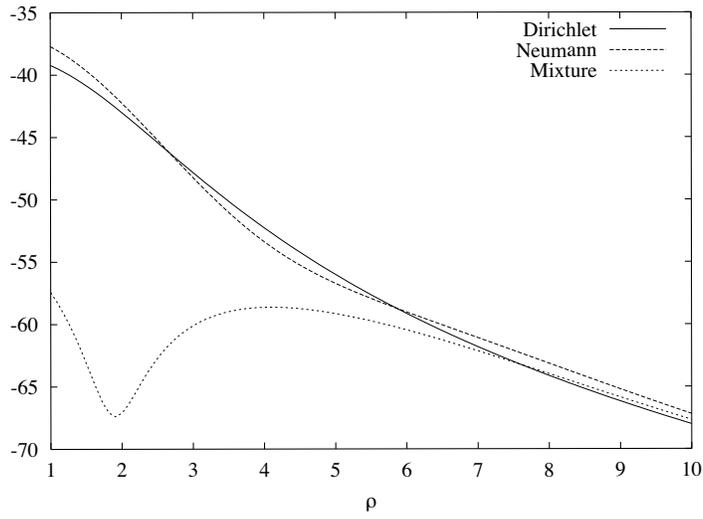


Figure 1. The absolute error (in dB) $|G_H(\rho, 1/2, 1/2) - G_{ArBC}(\rho, 1/2, 1/2)|$ in the Dirichlet, Neuman and Mixture cases.

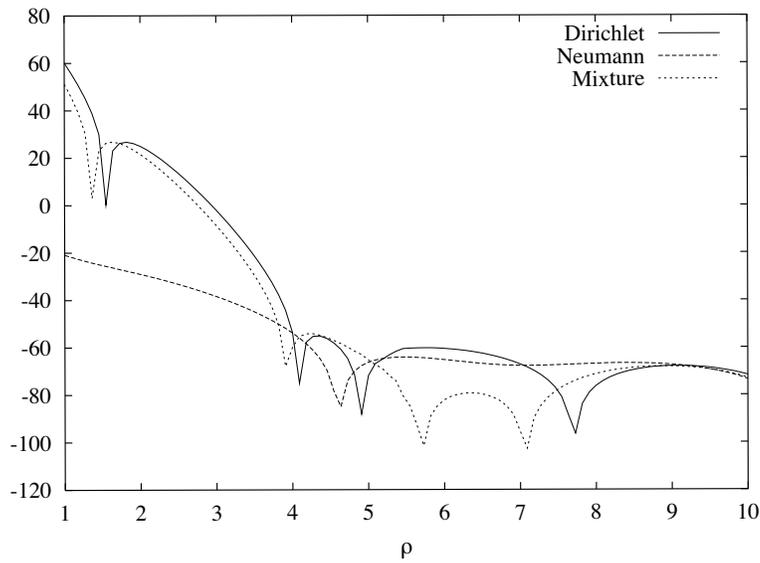


Figure 2. The absolute error (in dB) $|\Im[G(\rho, 1/2, 1/2) - G_{ArBC}(\rho, 1/2, 1/2)]|$ in the Dirichlet, Neuman and Mixture cases.

finite integral (evaluated with MATHEMATICA® NIntegrate) with integration variable $\gamma \in [0, 1]$, as seen in (91), we only compare the imaginary parts of the errors for the different approximations. The results are shown in Figure 2. It is seen that the Neumann ArBC is much better than the Dirichlet or mixture ArBC's up to $\rho \approx 5$, whereas for $\rho > 5$ the mixture ArBC tends to be better.

REFERENCES

1. Berenger, J. P., "A perfectly matched layer for the absorption of electromagnetic waves," *J. Comput. Phys.*, Vol. 114, 185–200, 1994.
2. Chew, W. C. and W. H. Weedon, "A 3-D perfectly matched medium from modified Maxwell's equations with stretched coordinates," *Microwave Opt. Technol. Lett.*, Vol. 7, 599–604, 1994.
3. Sacks, Z. S., D. M. Kingsland, R. Lee, and J. Lee, "A perfectly matched anisotropic absorber for use as an absorbing boundary condition," *IEEE Trans. Antennas Propagat.*, Vol. 43, 1460–1463, 1995.
4. Knockaert, L. and D. De Zutter, "On the stretching of Maxwell's equations in general orthogonal coordinate systems and the perfectly matched layer," *Microwave Opt. Technol. Lett.*, Vol. 24, 31–34, 2000.
5. Yuan, W. and E. P. Li, "Numerical dispersion and impedance analysis for 3d perfectly matched layers used for truncation of the fdtd computations," *Progress in Electromagnetics Research*, Vol. 47, 193–212, 2004.
6. Derudder, H., F. Olyslager, and D. De Zutter, "An efficient series expansion for the 2-D Green's function of a microstrip substrate using perfectly matched layers," *IEEE Microwave Guided Wave Lett.*, Vol. 9, 505–507, 1999.
7. Olyslager, F., "Discretization of continuous spectra based on perfectly matched layers," *SIAM J. Appl. Math.*, Vol. 64, 1408–1433, 2004.
8. Athanassoulis, G. A. and V. G. Papanicolaou, "Eigenvalue asymptotics of layered media and their applications to the inverse problem," *SIAM J. Appl. Math.*, Vol. 57, 453–471, 1997.
9. Sneddon, I. H., *The Use of Integral Transforms*, McGraw-Hill, New York, 1972.
10. Knockaert, L. F. and D. De Zutter, "On the completeness of eigenmodes in a parallel plate waveguide with a perfectly matched

- layer termination,” *IEEE Trans. Antennas Propagat.*, Vol. 50, 1650–1653, 2002.
11. Giraud, B. G. and K. Kato, “Complex-scaled spectrum completeness for pedestrians,” *Annals of Physics*, Vol. 308, 115–142, 2003.
 12. Newton, R. G., *Scattering Theory of Waves and Particles*, Second Edition, Springer-Verlag, New York, 1982.
 13. Boumenir, A., “Sampling and eigenvalues of non-self-adjoint Sturm-Liouville problems,” *SIAM J. Sci. Comput.*, Vol. 23, 219–229, 2001.
 14. Zayed, A. I., *Advances in Shannon’s Sampling Theory*, CRC Press, Boca Raton, FL., 1993.
 15. Chew, W. C., “A quick way to approximate a Sommerfeld-Weyl-type integral,” *IEEE Trans. Antennas Propagat.*, Vol. 36, 1654–1657, 1988.
 16. Arbenz, P. and M. E. Hochstenbach, “A Jacobi-Davidson method for solving complex symmetric eigenvalue problems,” *SIAM J. Sci. Comput.*, Vol. 25, 1655–1673, 2004.