The time domain discrete Green’s Function Method (GFM) characterizing the FDTD grid boundary

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Abstract

For a given FDTD simulation space with an arbitrarily shaped boundary and an arbitrary exterior region, most existing absorbing boundary conditions become inapplicable. A Green’s Function Method (GFM) is presented which accommodates arbitrarily shaped boundaries in close proximity to a scattering object and an arbitrary composition in the exterior of the simulation space. Central to this method is the numerical precomputation of a Green’s function tailored to each problem which represents the effects of the boundary and the external region. This function becomes the kernel for a single layer absorbing boundary operator. It is formulated in a manner which naturally incorporates numerically induced effects, such as the numerical dispersion associated with the FDTD scheme. The Green’s function is an exact absorber in the discretized space. This property should be contrasted to other methods which are initially designed for the continuum and are subsequently discretized, thereby incurring inherent errors in the discrete space which can not be eliminated unless the continuum limit is recovered. In terms of accuracy, the GFM results have been shown to be of a similar quality to the PML, and decidedly superior to the Mur condition. The properties of the GFM are substantiated by a number of numerical examples in one, two, and three dimensions.
I Introduction

With the advent of newly-introduced Absorbing Boundary Conditions (ABC's) for mesh truncation in the context of the Finite-Difference-Time-Domain (FDTD) computations, it has been recognized that the boundaries of the computational domain can be defined in close proximity to scatterers, and yet produce very small reflections. The most successful methods can be classified under two distinct categories: (a) approximations to the continuous one way wave equation at the boundary, e.g., the Engquist-Majda-Mur conditions [1], and (b) the use of artificial or physical absorbing materials near the boundary, such as the PML [2], [3]. It is typically assumed that the computational domain is bounded by a simple shape, e.g., a rectangular box or a sphere, which is embedded in free space. In some cases, it is also assumed that the waves impinging on the boundary are propagating, rather than evanescent waves. Most of these ABC's are initially formulated in the continuous domain, and then discretized for use in the FDTD scheme. Traditional ABC's of category (a), such as the Engquist-Majda-Mur conditions, are a discretized generalization of the continuous one-way wave equation. The one-way wave equation is basically equivalent in the continuum to an impedance relationship between the electric and magnetic fields. It is well known, though, that impedance relationships in the discretized world are different from the continuous ones, in view of the numerical dispersion that characterizes the discretized case. For this reason, adaptation of these conditions has been only partially successful, even when higher order approximations have been used. Significant experience has been generated recently with the application of category (b) ABCs such as the PML, which also relies on an initial continuous derivation. It is now recognized that several PML layers must be employed for sufficiently accurate results. This extra computational region imposes additional burden on the computational resources, particularly in 3D, compared with simpler methods that only need a small stencil close to the boundary.

The Johns matrix [4] was developed in the context of the TLM method as a Green's function representation of the external domain, and can be considered as an early attempt towards the formulation of an ABC along lines similar to this work. At the time of its development, though, it did not translate well into an accurate and efficient FDTD formulation. One can consider it as a spectral domain method in the sense that the waves are separated into incident and reflected waves at each removed branch leading to the boundary. The external medium is then viewed as a linear system, whose input and output are the incident and reflected waves, respectively. The impulse response of this system is pre-recorded for subsequent use in conjunction with the conventional TLM procedure. This method also features a means for a relaxation of the memory requirements by the usage of spatial interpolation in order to decrease the number of recorded branches. Further developments of this method have been carried out primarily in the context
of the TLM. Examples are refs. [5] and [6], where the Johns matrix has been used to extract frequency domain S-parameters of a specific region; ref. [7], where it was applied in 2-D and 3-D TLM formulations with artificial losses which provide an exponential drop-off as a means for further reducing the numerical reflections; and ref. [8], where the Johns matrix was developed as the Inverse Discrete Fourier Transform (IDFT) of the frequency domain modal S-parameters of a given network. Green’s functions in 1-D and 2-D have also been applied in the context of the FDTD algorithm in ref. [9] as ABC’s at the excitation plane. In this application, the temporal duration of the Green’s functions is set equal to the temporal length of the computations. Waveguide problems are treated on a modal basis for added efficiency in refs. [10] and [11]. Discrete and analytic Green’s functions are compared in ref. [12], where digital filters are used to eliminate unwanted high frequency components. An additional degree of efficiency, using Laguerre polynomials, was introduced in [13]. The Johns matrix is compared with other TLM, as well as FDTD, ABC’s in ref. [14].

The Green’s Function Method (GFM), described herein, was initially presented in [15]. As seen by the definitions of the inputs and outputs below, the GFM is formulated in the context of the inherently discretized spatial-temporal domain of the FDTD approach, rather than in the spectral domain. It provides a rigorous, inherently discrete, single layer boundary condition, whereby the effect of the external region has been replaced by the Finite Impulse Response (FIR) convolution summation over the boundary alone, in a diakoptic manner. This formulation features two terms for the tangential fields at the boundary, e.g., \( E = E_0 + E_1 \), where the first term, \( E_0 \), is an impedance-like relationship which couples the boundary field to field values at the closest space-time pixels within the computational domain. This term may be interpreted as an analog of the continuous one-way wave equation (see a frequency domain discrete generalization of this term in [16]). The second term, \( E_1 \), is generated by the process of discretization. It is a temporal FIR convolution summation with the Green’s function of the external region as its kernel. Being a phenomenon associated with the Yee discretization [17], this term includes the effects of numerical dispersion, thereby making the total expression for \( E \) exact in the discretized domain.

The derivation of the Green’s function involves no additional ansatz’s other than the fact that finite differences are being used and the external medium has known properties. In order to implement this ABC within the framework of the FDTD method, one needs to pre-compute the Green’s function for the specific boundary at hand and store it for the subsequent usage in the required convolution summation.

It should be stressed that the representation is quite general in that the external medium need not necessarily be free space, and the shape of the boundary is quite arbitrary (see a relatively
general boundary shape in Fig. 11). This allows for the boundary to conform to the region of interest. As an example, one can select a computational domain with a minimal “white space” for the inclusion of a certain scatterer (or a family of scatterers) and pre-calculate the appropriate Green’s function for the boundary of this domain.

The properties of the GFM are substantiated by a number of numerical examples in one, two, and three dimensions. The development of the method is presented in one dimension first, for the sake of simplicity, in Section II. The two and three dimensional discrete Green’s functions are cast in the form of a matrix containing the impulse response of each boundary point as well as the relationships between any two points, as discussed in Sections III and IV, respectively. The matrix being used for calculating the $3 - D$ boundary field values at each time step is based on the historical values at this and several adjacent boundary points. Due to the quasi-local nature of the Green’s function and because only one layer is involved, this matrix is very sparse; hence, the convolution operation is quite efficient. The examples worked out for these cases attest to the fact that significant improvement is achieved in the level of reflection errors over the traditional Engquist-Majda-Mur ABC, and the quality of the results is comparable to the Perfectly Matched Layers (PML)-type boundary conditions. Finally, conclusions are drawn in Section V.

II One dimensional Green’s function

The impedance and FIR terms introduced above are easily recognized in the one dimensional case, where the space–time grid is defined as $t = n\Delta t$ and $x = i\Delta x$, with the Courant–Friedrich–Levy (CFL) number $\gamma = c\Delta t / \Delta x$. The direction of propagation is assumed here to be $+x$, and the electromagnetic field is comprised of the $E_z$ and $H_y$ components. For the sake of simplicity, a normalized magnetic field $\sqrt{\varepsilon \mu} H$ is used throughout and renamed $H$. Each field sample is linked to three other samples in the manner required by the Yee algorithm, e.g., for the four neighboring space-time values the FDTD scheme reads

$$E_z^{n+1}(i) = E_z^n(i) + \gamma[H_y^{n+\frac{1}{2}}(i + \frac{1}{2}) - H_y^{n+\frac{1}{2}}(i - \frac{1}{2})]$$

(1a)

$$H_y^{n+\frac{1}{2}}(i + \frac{1}{2}) = H_y^{n-\frac{1}{2}}(i + \frac{1}{2}) + \gamma[E_z^n(i + 1) - E_z^n(i)]$$

(1b)

The general formulation involves a medium $\Gamma$ surrounded by the boundary $\partial\Gamma$. In this case, the computational domain is $\Gamma = [x; 0 \leq x \leq I\Delta x]$, where the plane $x = 0$ contains the excitation, hence $\partial\Gamma = [x; x = I\Delta x]$. We also define the external region as $\Gamma = [x; x \geq (I + \frac{1}{2})\Delta x]$ (see Fig. 1).

We now apply Eqns. (1) over the internal and external regions separately. For each region one
can define a boundary term which facilitates the coupling to the other region. The boundary term for the internal problem is described, using Eq. (1a) at \( \partial \Gamma \), by

\[
E_z^{n+1}(I) = -\gamma H_y^{n+\frac{1}{2}}(I - \frac{1}{2}) + E_z^n(I) + \gamma H_y^{n+\frac{1}{2}}(I + \frac{1}{2})
\]  

(2)

We wish to solve Eq. (2) in order to find \( E_z^{n+1} \) on the boundary of \( \Gamma \). Eq. (2) can also be reinterpreted as

\[
E_z^{n+1}(I) = -\gamma H_y^{n+\frac{1}{2}}(I - \frac{1}{2}) + E_z^n(I) + \gamma H_y^{n+\frac{1}{2}}(I + \frac{1}{2}) \left( \underbrace{E_{0z}^{n+1}}_{\text{E_{0z}^{n+1}}} \right) \left( \underbrace{E_{1z}^{n+1}}_{\text{E_{1z}^{n+1}}} \right)
\]  

(3)

The interior “impedance term” \( E_{0z}^{n+1} \) and the unknown term \( E_{1z}^{n+1} \) are defined herein. We solve for \( E_{1z}^{n+1} \) by defining a boundary value problem within \( \Gamma \), where \( E_z^n(I) \) is the boundary value representing the effect of \( \Gamma \) on the computation in \( \Gamma \). This term reappears in \( \gamma H_y^{n+\frac{1}{2}}(I + \frac{1}{2}) \) as follows:

\[
H_y^{n+\frac{1}{2}}(I + \frac{1}{2}) = H_y^{n+\frac{1}{2}}(I + \frac{1}{2}) + \gamma[E_z^n(I + 1) - E_z^n(I)]
\]

(4)

The boundary term \( E_z^n(I) \), now viewed as an excitation for \( \Gamma \), can be decomposed into a set of arbitrary functions in view of the linearity of the problem. If these functions are impulsive, i.e.,

\[
E_z^n(I) = \begin{cases} 
1 & \text{for } n = 0 \\
0 & \text{for } n \neq 0 
\end{cases}
\]

(5)

then the region \( \Gamma \) is characterized by a discrete temporal Green’s function represented by the series \( G^n, n = 1, 2, \ldots \) which relates \( E_{1z} \) as the output to a general input \( E_z \). The impulsive function (5) is used as the excitation for an FDTD computation over \( \Gamma \) in order to evaluate \( G^n \). This Green’s function now provides the mechanism for treating any temporal dependence of \( E_z^n(I) \) via a discrete convolution relationship with the historical field values at \( \partial \Gamma \):

\[
E_{1z}^{n+1}(I) = \sum_{j=1}^{\infty} G^j E_z^{n+1-j}(I) \triangleq G^n * E_z^{n+1}(I)
\]

(6)

where we use the standard definition of the discrete convolution \(* \) noting that \( G^n = 0 \) for \( n \leq 0 \). Note also that the summation in (6) may be truncated at \( j = n + 1 \) in view of the zero initial condition for \( n < 0 \). In this way, Eq. (3) becomes

\[
E_z^{n+1}(I) = -\gamma H_y^{n+\frac{1}{2}}(I - \frac{1}{2}) + G^n * E_z^{n+1}(I)
\]

(7)
Equation (7) is the GFM ABC.

Note that \( G^n \) depends only on the composition of the external medium \( \Gamma \) and the sampling intervals (and, hence, on \( \gamma \)); it does not depend on the actual excitation. It thus applies to any problem and may be pre-computed for subsequent use with many different FDTD computations within \( \Gamma \). The exact Green’s function \( G^n \) is truncated to order \( N \). As seen below, an important property of \( G^n \) is its rapid decay with \( n \). Therefore, the FDTD computation, as described above, need not penetrate deeply into \( \Gamma \).

The term \( E_{0z}^{n+1}(I) = -\gamma H_y^{n+1/2}(I - 1/2) \) in Eq. (3) can be seen as an impedance relationship, analogous to the continuous one-way wave equation. To see this analogy, we resolve the continuous wave solution in \( \Gamma \) into two constituents, viz. \( \mathbf{\hat{E}} \) and \( \mathbf{\hat{E}} \), which propagate in the \( +x \) and \( -x \) directions, respectively. In the continuous limit, these two constituents can be found at any \( x \) from the total electromagnetic field \( (\mathbf{E}, \mathbf{H}) \) via

\[
\mathbf{\hat{E}} = \frac{1}{2}(\mathbf{E} - \hat{x} \times \mathbf{H}), \quad (8a)
\]
\[
\mathbf{\hat{E}} = \frac{1}{2}(\mathbf{E} + \hat{x} \times \mathbf{H}) \quad (8b)
\]

Ideally, one could use (8) to eliminate reflections from \( \partial \Gamma \) by setting \( \mathbf{\hat{E}} = 0 \), i.e., by utilizing the condition

\[
\mathbf{E} = -\hat{x} \times \mathbf{H} \quad (9)
\]
as an ABC for the continuous limit. A discretization of this continuous ABC is, in fact, the first term in (7). However, note that this expression alone does not suffice as the discrete domain ABC as expressed in (7), except in the CFL-stability limit of \( \gamma = 1 \) (where no numerical dispersion is present). It is also equivalent to the first order Mur condition, which is exact in that case. The term \( E_{1z}(I) \) in (7) is generated by the process of discretization. Being a phenomenon associated with the Yee discretization, this term includes the effects of numerical dispersion, thereby making the total expression for \( \mathbf{E}_z(I) \) exact in the discrete domain.

II.A Evaluation of the Green’s Function in 1D: \( \Gamma = \text{Free Space} \)

We follow the process described above to compute the free space, 1-D, \( \gamma \)-dependent series \( G^n \). Both the input \( E_z(I) \) and output \( E_{1z}(I) \) are defined at \( \partial \Gamma \). Applying the unit temporal impulse of (5) as an input at \( \partial \Gamma \), the output is the Green’s function \( G^n = E_{1z}^n(I) \) for \( n \geq 1 \) (recall that \( E_{1z}^n(I) = 0 \) for \( n \leq 0 \)). Substituting Eq. (4) into Eq. (2), we obtain

\[
E_{z}^{n+1}(I) = -\gamma H_y^{n+1/2}(I - 1/2) + E_{0z}^n(I) - \gamma^2 E_{1z}^n(I) + ... \quad (10)
\]
Using Eqs. (1) repeatedly, \( E_{1z} \) at \( \partial \Gamma \) can be further expanded as:

\[
E_{1z}^{(n+1)}(I) = (1 - \gamma^2) E_{1z}^n(I) + (-\gamma^2 + \gamma^4) E_{1z}^{n-1}(I) + (-\gamma^2 + 3\gamma^4 - 2\gamma^6) E_{1z}^{n-2}(I) + \ldots \tag{11}
\]

which gives the series \( G^n \) as:

\[
G^n = 1 - \gamma^2,
-\gamma^2 + \gamma^4,
-\gamma^2 + 3\gamma^4 - 2\gamma^6,
-\gamma^2 + 6\gamma^4 - 10\gamma^6 + 5\gamma^8,
-\gamma^2 + 10\gamma^4 - 30\gamma^6 + 35\gamma^8 - 14\gamma^{10}, \ldots
\tag{12}
\]

Note that all coefficients in (12) include products of \( (1 - \gamma^2) \). Therefore, in the stability limit \( \gamma = 1, \) \( G^n = 0, \ldots \), and this expression coincides with the one way equation or the first order Mur ABC. The entries of \( G^n \) drop off quite rapidly; e.g., \( G^n = 0.51, -0.2499, -0.0050, 0.0624, \ldots \) for \( \gamma = 0.7 \). This rapid temporal decay of the successive terms in \( G^n \), indeed renders the evaluation of \( E_{1z}(I) \) via the convolution integral in Eq. (7) a quasi-local operation.

### II.B Analytic Expressions for the Frequency Domain Green’s Function

The time dependence in the difference equations (1) can be transformed into a frequency dependence via the \( z \)-transform which is defined for a causal function \( x(n) \) as (using \( w \) as the spectral variable rather than \( z \)):

\[
\tilde{X}(w) = Z\{x\} \triangleq \sum_{n=0}^{+\infty} x(n) \, w^{-n}
\tag{13}
\]

A \( z \)-transform of Eq. (7) renders the temporal convolution a multiplicative operation in the frequency domain.

For symmetry reasons, it is convenient to define the \( z \)-transforms, normalizing the magnetic field, as follows:

\[
\tilde{H_y}(w, i) = Z\{H_y^n(i)\}
\tag{14a}
\]

\[
\tilde{E_z}(w, i) = Z\{E_z^n(i)\}
\tag{14b}
\]

\[
\tilde{G}(w) = Z\{G^n\}
\tag{14c}
\]

Thus, the transform of (1) is

\[
\tilde{E_z}(w, i) w^{-1} = \tilde{E_z}(w, i) + \gamma \left[ \tilde{H_y}(w, i + \frac{1}{2}) w^{-\frac{1}{2}} - \tilde{H_y}(w, i - \frac{1}{2}) w^{-\frac{1}{2}} \right]
\tag{15a}
\]

\[
\tilde{H_y}(w, i + \frac{1}{2}) w^{-\frac{1}{2}} = \tilde{H_y}(w, i + \frac{1}{2}) w^{\frac{1}{2}} + \gamma \left[ \tilde{E_z}(w, i + 1) - \tilde{E_z}(w, i) \right]
\tag{15b}
\]
In order to develop a closed form expression for \( \tilde{G} \) we make use of the concepts of the discrete-frequency domain trans-impedance and trans-admittance as defined in [16]. The trans-impedance \( \tilde{Z}_i(\gamma; w) \) is defined for a wave propagating toward the boundary in the \(+x\) direction as the ratio between the electric and magnetic field samples at the points \( i \) and \( i - \frac{1}{2} \), respectively, their respective adjacent locations within the Yee grid:

\[
\tilde{Z}_i(w) = \frac{\tilde{E}_z(w, i)w^{-1/2}}{\tilde{H}_y(w, i - \frac{1}{2})}
\]  
(16)

Similarly, the trans-admittance for the same wave is defined as

\[
\tilde{Y}_{i+1/2}(w) = \frac{\tilde{H}_y(w, i + \frac{1}{2})w^{-1/2}}{\tilde{E}_z(w, i)}
\]  
(17)

In order to evaluate these concepts in closed form at some point \( i \), we make use of the block diagram in Fig. 2, which is a linear system representation of the \( z \)-transform of the Yee grid. In particular, Eqs. (15a)–(15b) are represented in this figure by the blocks between the lines \( a - a \) and \( b - b \), and between \( b - b \) and \( c - c \), respectively. Taking the line \( a - a \) as a representation of the plane \( i \), we note that \( \tilde{H}_y(w, i - \frac{1}{2})w^{-1/2} \) and \( \tilde{E}_z(w, i)w^{-1} \) appear there as an input and output, respectively, for the entire system, with the transfer function \( \tilde{Z}_{a-a}(w) = \tilde{Z}_i(w) \). Taking the line \( b - b \) on the other hand, then \( \tilde{E}_z(w, i) \) and \( \tilde{H}_y(w, i + \frac{1}{2})w^{-1/2} \) are the input and output, with the transfer function \( \tilde{Y}_{b-b}(w) = \tilde{Y}_{i+1/2}(w) \). In principle, one would have to take into account an infinite number of blocks to obtain these transfer functions. Alternatively, we make use of Eq. (15a) with (16)-(17) to obtain:

\[
\tilde{Z}_i(w) = w\tilde{Z}_i(w) + \gamma \left( \tilde{Y}_{i+1/2}(w)\tilde{Z}_i(w) - 1 \right)
\]  
(18)

Equations (15a) and (15b) are dual to each other, a fact that makes the blocks \( a - a \) to \( b - b \) and \( b - b \) to \( c - c \) identical, as seen in Fig. 2. As a result, the two expressions (16)-(17) are also identical, therefore a common definition of a transfer function \( \tilde{G}_0 \) can replace both the trans-impedance and the trans-admittance as follows:

\[
\tilde{G}_0 = \tilde{Z}_i = \tilde{Y}_i
\]  
(19)

This transfer function is obtained from (18) and (19) and has the following form:

\[
\tilde{G}_0(w) = \frac{1 - w - \sqrt{(1 - w)^2 + 4\gamma^2w}}{2\gamma w}
\]  
(20)

In order to define the branches of the square root operator we rewrite (20) as

\[
\tilde{G}_0(w) = \frac{1 - w - \sqrt{(w - w_1)(w - w_2)}}{2\gamma w}
\]  
(21)
with the branch points defined as

\[ w_{1,2} \equiv 1 - 2\gamma^2 \pm j2\gamma\sqrt{1-\gamma^2} \tag{22} \]

Both branch points are located on the unit circle, provided that \( \gamma \leq 1 \). Defining the principal branch, for both \( \sqrt{w-w_1} \) and \( \sqrt{w-w_2} \), as \(-\pi/2 < \arg(w-w_{1,2}) < 3\pi/2\), the branch cuts are selected as shown in Fig. 5. With this choice, the transfer function becomes analytic outside the unit circle, and this condition ensures causality.

Using the \( z \)-transform of (7) and (16), \( \tilde{G} \) can be expressed in terms of \( \tilde{G}_0 \):

\[ \tilde{G}(w) = w^{-1} \left( 1 + \frac{\gamma}{\tilde{G}_0(w)} \right) \tag{23} \]

or with the help of Eq. (18),

\[ \tilde{G}(w) = 1 + \gamma \tilde{G}_0(w) \tag{24} \]

where \( \tilde{G}(w) = z \left[ \tilde{G} \mid N \to \infty \right] \), and \( G \) appears after (6). Note that if \( \gamma = 1 \), \( \tilde{G}_0(w) = -1 \), which leads to \( \tilde{G}(w) = 0 \). Additionally, note that causality is satisfied:

\[ \lim_{w \to \infty} G(w) = 0 = G^n, \quad n \leq 0 \]

and the initial value theorem agrees with (12):

\[ \lim_{w \to \infty} wG(w) = 1 - \gamma^2 = G^1 \]

Transforming the variable \( w \) into the Fourier variable \( \Omega \), i.e., \( w = \exp j\Omega \), where \( \Omega = \omega \Delta t/2 \), we have from Eq. (20)

\[ \tilde{G}_0(\Omega) = \frac{-j \sin \Omega + \sqrt{\gamma^2 - \sin^2 \Omega}}{\gamma \exp j\Omega}. \tag{25} \]

This result is identical to the frequency domain FDTD development in [16].

The expression in Eq. (25) shows that one can distinguish between a low and high frequency range, respectively, below and above the cutoff frequency defined by \( \gamma^2 - \sin^2 \omega \Delta t = 0 \). In the low frequency range, the magnitude can be expressed as \( |\tilde{G}_0(\Omega)| = 1 \). This constant value indicates an impedance matched medium for all frequencies below cutoff. The phase in the lower range is monotonically decreasing, where in the limit \( \Omega \to 0 \), i.e., either the continuous limit \((\Delta t \to 0)\) or the very low frequency limit \((\omega \to 0)\), a linear phase delay is observed: \( \angle \tilde{G}_0(\Omega) \approx \pm \frac{\Omega}{\gamma} \). As the frequency increases, the delay becomes frequency dependent due to numerical dispersion, and the phase velocity drops until it reaches the value of zero at the cutoff frequency. In the high frequency
(stop band) range, we have a linearly increasing phase, with a frequency dependent magnitude. In this region, no propagation is possible. Indeed, traces of high frequency components are known to be trapped behind propagating pulses in FDTD simulations. This cutoff phenomenon is seen in Figures (3),(4) for the amplitude and phase behavior of $\tilde{G}_0(\Omega)$, respectively. The cutoff condition implies $\Delta x < \frac{1}{2\pi}$ (assuming $\Omega \ll 1$), and is usually satisfied in conventional FDTD implementations.

**Truncation Effects:** The accuracy of the solution depends on the order of the approximation of $\tilde{G}$, denoted by $N$; $N$ is the size of the rectangular window $H(\exp(j\omega))$ by which the exact Green’s function is filtered\(^1\).

$$H(e^{j\omega}) = e^{j\omega \frac{\pi}{4} \frac{\sin[\omega(N + 1)/2]}{\sin[\omega/2]}}$$ \hspace{1cm} (26)

By using a finite number of coefficients in this window, the exact frequency domain function of Eq. (26) is smeared over a frequency band. An example of the frequency domain form of a truncated Green’s function is shown in Fig. 6.

**II.C The merits of the 1-D GFM in comparison with the Mur and PML ABCs**

**II.C.1 Numerical Efficiency**

Eq. (7) involves $N$ multiply-add operations in addition to the regular FDTD operations (recall that $N$ denotes the order of approximation).

In the First Order Mur method, we use the following formula to calculate the field at the next timestep at the boundary:

$$E_z^{n+1}(I) = E_z^n(I - 1) - \frac{1 - \gamma}{1 + \gamma} [E_z^{n+1}(I - 1) - E_z^n(I)]$$ \hspace{1cm} (27)

Therefore, for the First Order Mur method, one needs to perform one multiply-add operation only in addition to the regular FDTD operations. In this sense, the Mur method is advantageous, however, as seen below, this advantage becomes less significant in two and three dimensions, especially in view of the fact that the GFM can produce more accurate results. Note also that when $\gamma = 1$, the first order Mur and the GFM indeed coincide.

Turning to the PML method, we have the basic relations as follows [2]:

$$\epsilon_0 \frac{\partial E_z}{\partial t} + \sigma E_z = \frac{\partial H_y}{\partial x}$$ \hspace{1cm} (28a)

$$\mu_0 \frac{\partial H_y}{\partial t} + \sigma^* H_y = \frac{\partial E_z}{\partial x}$$ \hspace{1cm} (28b)

\(^1\)Windows other than rectangular can be utilized. In fact, our numerical examples below show that improved accuracy can be achieved with smoother windows such as the Hanning window (see Section II.C.3).
For simplicity, we use $\epsilon_0 = \mu_0 = 1$ and $\sigma = \sigma^*$. Discretizing all derivatives by their linear approximations, we have

\[
E_i^{n+1} = \frac{\gamma}{1 + \beta} [H_i^{n-1/2}] + \frac{1 - \beta}{1 + \beta} E_i^n
\]

\[
H_{i+1/2}^{n+1/2} = \frac{\gamma}{1 + \beta} [E_{i+1}^n - E_i^n] + \frac{1 - \beta}{1 + \beta} H_{i+1}^{n+1/2}
\]

(29a)

with $\beta \equiv \frac{\sigma \Delta t}{2}$. Here, each time step requires $2L$ multiplication operations and $3L$ summations in additional to the regular FDTD operations, where $L$ is the number of layers. Therefore, numerical comparisons between the PML and the GFM will be conducted under the condition of equal complexity, i.e., $N = 2L$. Interestingly, note that in the case were $\beta = 0$ and $\gamma = 1$, these expressions, too, reduce to the GFM formulation.

### II.C.2 Stability

The GFM stability is studied extensively in [19]. Stability of the GFM is dependent, in general, on the composition of the internal domain and on the shape and nature of the boundary. By transforming the GFM formulation into matrix form, which allows for an eigenvalue analysis, stability criteria are derived in [19] as extensions of the CFL rule. In this context, all one dimensional cases treated so far have shown stable characteristics.

### II.C.3 Accuracy

A criterion for accuracy is the reflection coefficient at the boundary. The reflection is computed with comparison to a case of a larger grid which extends beyond the boundary and thus enables a longer time span of reflectionless propagation for a given pulse. The value of the reflection coefficient is dependent upon the definition of the error, therefore the results herein should be interpreted only in the comparative sense. A one dimensional example, worked out with a Green's function with $N = 20$ terms, and using a trapezoidal excitation with $\gamma = 0.5$, has yielded a return loss of $-45$ dB. When the Green's function was tapered with a Hanning window instead of rectangular window, the return loss improved to the level of $-55$ dB. The same problem, when worked out with the First Order Mur method, yields $-43$ dB return loss using the same error definition as in the GFM. A representative PML with parabolic profile and $L = 10$ layers has been also used for this problem. It should be noted that from the point of view of complexity, $L = 10$ layers are equivalent to $N = 20$ terms in the GFM. The PML reflection error is $-55$ dB. We can thus see that the GFM, when enhanced with the Hanning window, outperforms the First Order Mur method, and is equivalent to the PML for a given computational load.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>GFM</th>
<th>First Order Mur</th>
<th>PML</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical complexity</td>
<td>( N ) multiply-add operations</td>
<td>one multiply-add operation</td>
<td>( 2L ) multiplications</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( 3L ) summations</td>
</tr>
<tr>
<td>Stability</td>
<td>Stable</td>
<td>Stable</td>
<td>Stable</td>
</tr>
<tr>
<td>Reflection error</td>
<td>-45 dB</td>
<td>-43 dB</td>
<td>-55 dB</td>
</tr>
<tr>
<td>with ( \gamma = 0.5 )</td>
<td>-55 dB</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Programming complexity</td>
<td>fair</td>
<td>low</td>
<td>complex</td>
</tr>
</tbody>
</table>

Table 1: Comparison summary for the one dimensional case

II.C.4 Comparison summary

The results of the GFM, as compared with the First Order Mur and PML methods, with \( N = 20 \) and \( L = 10 \) PML layers, are summarized in Table (1). One can see that the GFM is on par with existing methods, and in particular it is comparable to the PML. However, as mentioned in the Introduction, a main advantage of the GFM is its generality and flexibility, since it allows for boundaries with arbitrary shapes, and the external medium can be of arbitrary composition. These properties can be seen more clearly in the two and three dimensional cases described in Sections III and IV.

III Two Dimensional Case

III.A Algorithm Description

Consider a region \( \Gamma \) in the two dimensional space \( x-y \), bounded by a contour \( \partial \Gamma \), which can have an arbitrary shape as shown in Fig. 7. The contour consists of \( M \) field grid points, each with its own coordinates \((x_1, y_1), (x_2, y_2), \ldots, (x_M, y_M)\). The choice of boundary points depends on the geometry of the problem and is made in such a way that the white space will be minimized and that only one type of field will be included. General types of boundaries, with dual expressions for the both electric and magnetic boundary field samples, can be accommodated with a similar derivation. This derivation is detailed in [19].

For the sake of simplicity, we first focus on a TE\(_x\) wave with the components \( E_z, H_y \) and \( H_x \), and consider that part of the boundary \( \partial \Gamma \) that absorbs wave propagating in the \(+x\) direction. The \( M \) boundary points on \( \partial \Gamma \) are selected as \( H_y \) field components where the \#\( m \) point denoted as \( H_y(m) \) represents \( H_y(x_m, y_m) \). Similarly to the 1-D case (Equation (7)), the 2-D GFM features
two terms for the field at the boundary, i.e., the field at a given point \( m \) is expressed as

\[
H_{y}^{n+1}(m) = -\gamma_x E_z^{n+1/2}(m) + \sum_{m'=1}^{M} \sum_{j=1}^{N} G^j(m,m') H_{y}^{n+1-j}(m')
\]

\[
G^{n+1}(m,m') \ast H_{y}^{n+1}(m')
\]

where the convolution is defined in (6), and \( \gamma_x = c \frac{\Delta t}{\Delta x} \). Equation (30) can be recast in a vector format:

\[
\begin{aligned}
H_{y}^{n+1} &= -\gamma_x E_z^{n+1/2} + G^{n+1} \ast H_{y}^{n+1} \\
&= \begin{pmatrix}
H_{0y}^{n+1} \\
H_{iy}^{n+1}
\end{pmatrix} + \begin{pmatrix}
H_{0y}^{n+1} \\
H_{iy}^{n+1}
\end{pmatrix}
\end{aligned}
\]

where the star operator denotes a temporal convolution performed concurrently with a spatial matrix multiplication, while spatial vectors and dyads are denoted by an underline and double underline, respectively.

The first term in (31) \( \frac{H_{0y}^{n+1}}{H_{iy}^{n+1}} \) is an impedance-like term as in (7) while the second term \( \frac{H_{iy}^{n+1}}{H_{iy}^{n+1}} \) involves the temporal-spatial dyadic Green’s function \( G^m \). A representative dyadic element \( G^m(m,m') \) corresponds to the FDTD calculated response at the point \( m \) on the boundary to an impulsive excitation, \( t = n \Delta t \) earlier, at the point \( m' \) defined at \( \partial \Gamma \). Consequently, one must use \( M \) simulations to construct the dyadic series \( G^m \). Once incorporated in the convolution operator in (31), this dyad transforms backstored values over the boundary to the next timestep.

This formulation is reduced to the 1-D case (7) by setting \( M = 1 \). The size of the matrix used to store the dyadic series \( G^m \) determines the efficiency of the GFM. As demonstrated in the examples below, this matrix has a short temporal duration as well as a compact spatial extent.

### III.B Two dimensional examples

#### III.B.1 Two dimensional waveguide problem

The first 2D examples deals with a Perfect Magnetic Conductor (PMC) parallel-plate waveguide in the \( x-y \) plane. The waveguide is excited at the plane \( x = 0 \) by a TE\(_x\) field which has no variations in the \( z \) direction, and is either a trapezoidal pulse or a harmonic wave. The corresponding lattice is given in Fig. 8.

The Green’s dyad \( G^m \) is defined at the plane \( \partial \Gamma = [x; x = x_{max}] \). In accordance with the philosophy of the GFM as described above, \( G^m \) serves to represent the waveguide region beyond \( \partial \Gamma \). In order to evaluate this function, we excite each cell on \( \partial \Gamma \) by a temporal impulse independently and record the values of the output \( H_{iy} \) over \( \partial \Gamma \). For the case of \( \gamma_x = \gamma_y = 0.5 \), \( N = 20 \) and \( M = 4 \), some numerical values of \( G^m \) are shown in Table 2. Each block in Table 2 describes entries
Table 2: Numerical values for the two-dimensional Green's function at \( x = x_{\text{max}} \). \( \gamma_x = \gamma_y = 0.5 \), \( N = 20 \) and \( M = 4 \).

\[
\begin{array}{cccccc}
\text{Excitation} & t = n + 1 & t = n + 2 & t = n + 3 & \ldots \\
\hline
\) & Output & Cell & Output & Cell & Output & Cell \\
1 & 0.75 & 0 & 0 & 0 & -0.125 & -0.0625 & 0 & 0 & +0.0313 & -0.1094 & -0.0156 & 0 & \ldots \\
2 & 0 & 0.75 & 0 & 0 & -0.0625 & -0.0625 & -0.0625 & 0 & -0.1094 & 0.1250 & -0.0838 & -0.0156 & \ldots \\
3 & 0 & 0 & 0.75 & 0 & -0.0625 & -0.0625 & -0.0625 & -0.0625 & -0.0156 & -0.0038 & 0.125 & -0.1004 & \ldots \\
4 & 0 & 0 & 0 & 0.75 & 0 & 0 & -0.0625 & -0.125 & 0 & -0.0156 & -0.1004 & 0.0313 & \ldots \\
\end{array}
\]

of \( G^n \) across a certain time interval for all \( M \times M \) excitation and response points over \( \partial \Gamma \). The shortest time interval is represented by the leftmost block \( (t=n+1) \) which is diagonal, reflecting the fact that the signal from each excitation cell has not propagated yet to neighboring cells. These diagonal values are equal to \( 1 - \gamma^2 \). The second block, for which \( t=n+2 \), has a main diagonal and two sub-diagonals, due to propagation up to the adjacent cells. Additional sub-diagonals are added at each subsequent time interval, resulting in more populated blocks with block-diagonal structure, as can be seen in the Table. The total number of blocks is \( N \). Note also that entries of \( G^n \) decrease in magnitude as their position becomes farther away from the main diagonal, and as the time interval increases. These behaviors allow for a fairly early truncation of the matrix. In this example, \( M \) is rather small, therefore the computations have been performed with a relatively larger \( N \). Generally, though, \( M \) may become quite large, such that \( N \ll M \). In cases like these, all \( N \) blocks will have the block-diagonal structure with no more than \( 2N+1 \) diagonals in each block, and the matrix would indeed be quite sparse.

Using the GFM with the Green's function as computed herein, TE\(_0\) mode propagation was simulated in a waveguide 25 cells long, and the results for the first 200 time steps were compared with those of a waveguide 225 samples long. A very good match has indeed been obtained. The reflection error was 20 dB below that obtained with the Mur method.

In order to observe the effect of the order of approximation on the accuracy of the results, a reference problem was first created by embedding the basic structure in a relatively large \((9 \times 225)\) grid, such that no reflections arise within the first 200 timesteps. The order of the temporal GFM approximation was set from \( N = 1 \) to \( N = 20 \), and the return loss with respect to the reference solution was calculated. The results for \( \gamma = 0.7 \) are shown in Fig. 9. As expected, the higher the order of approximation, the more accurate the results are (note, again, that the reflection values in Fig. 9 are valid only in a comparative sense).
III.B.2 A waveguide with an obstacle

Next we have placed a metallic obstacle within the parallel plate waveguide. The location of this obstacle in \( \Gamma \) with respect to the absorbing boundary, \( X_{wall} \), was changed within the range of ten cells to one cell in order to examine the effect of the proximity of this scatterer to the boundary. Fig. 10 shows the the return loss for the different boundary-to-obstacle distances, for the case \( \gamma = 0.7, N = 20, M = 4 \). These results make it clear that the absorbing boundary can be placed in very close proximity to the scattering object with almost no influence on the reflection loss.

III.B.3 A waveguide with a sawtooth–like boundary

As mentioned above, although the example in Section III.B.1 was solved with \( \partial \Gamma \) being a plane, the GFM can easily support arbitrary geometries of the boundary as well. To illustrate this feature, a parallel plate waveguide, similar to the one analyzed in Section III.B.1, is terminated with a sawtooth–like boundary (see Fig. 11). The GFM now requires the recording of two field components at the boundary, since the boundary no longer conforms to a plane with a single field component. The application of the GFM is straightforward nonetheless. As seen in Fig. 11, the field within the waveguide is a sinusoid, representing a propagating wave in the \( x \)-direction, even though the waveguide is truncated by the sawtooth-shaped boundary. The measured reflection error is \(-28 \text{ dB}\). This result is in fact \( 3 \text{ dB} \) lower than the one obtained with the GFM for the same basic configuration with a planar boundary. A comparison with other methods is not feasible in this case due to the complexity of the boundary shape.

It should be noted that the Green’s function has been evaluated specifically for this boundary shape. In fact, the entire operator is dependent upon the boundary shape, and the issue of stability is also closely associated with it. This shape determines the value of \( \gamma \) allowed for stable computations, which may be lower than the one required by the intrinsic FDTD algorithm (see discussion in Sec. III.C.2). The fact that irregular boundary shapes like the one in Fig. 11 can be handled with almost the same complexity as simple boundaries sets the GFM apart from such methods as Mur and PML.

III.B.4 Two dimensional free space excited through an aperture

In this example, the GFM is applied over the three walls \( x = x_{max}, y = 0, y = y_{max} \) in free space. The fourth wall, \( x = 0 \) is a PMC with an aperture cut in it, containing the excitation. The geometry of the problem is shown in Fig. 12. Assuming \( M = 50 \) and \( N = 10 \), the elements in the matrix containing \( G \) are grouped in 10 blocks \( 50 \times 50 \) each, or a total of 25,000 entries (see the
matrix structure explanation in Section III.B.1 in regards to Table 2). Only 18% of these entries are non-zero. This very sparse matrix structure is indicative of the relatively modest memory requirements associated with the GFM. The results are summarized in Table 3.

III.C  Merits of the 2-D GFM in comparison with the Mur and PML methods

III.C.1  Numerical efficiency

Consider the 2-D GFM, as expressed in Eq. (30). The arithmetic operations in this equation involve the multiplication of the $M \cdot N$ vector containing $H_y$ by the $M \cdot N \times M$ matrix $\bar{G}$, of the form shown in Table 2 at each time step. The total multiply-add operations count, therefore, $M^2 \cdot N$, in addition to the regular FDTD operations. However, since $\bar{G}$ is represented as a sparse matrix (see Table 2), this computational cost can be significantly reduced, especially for long boundaries having $M >> N$. Since each block in Table 2 contains no more than $N$ sub-diagonals, reflecting the fact that each boundary point interacts with its $N$ neighbors only, the total operation count is reduced to $M \cdot N^2$.

The Mur ABC is represented at each boundary point as follows:

$$H^{n+\frac{1}{2}} \left( I + \frac{1}{2} \right) = H^{n+\frac{1}{2}} \left( I - \frac{1}{2} \right) - \frac{1 - \gamma}{1 + \gamma} \left[ H^{n+\frac{1}{2}} \left( I - \frac{1}{2} \right) - H^{n-\frac{1}{2}} \left( I + \frac{1}{2} \right) \right].$$

(32)

This formula involves one multiply-add operation per timestep, in addition to the regular FDTD operations.

For the sake of comparison with the PML ABC, consider a simple case where $\epsilon_0 = \mu_0 = 1$ and $\sigma = \sigma^*$. The 2-D PML TM equations are [18]:

$$\begin{align*}
\epsilon_0 \frac{\partial E_{xx}}{\partial t} + \sigma_x E_{xx} &= \frac{\partial H_y}{\partial x} \quad \text{(33a)} \\
\epsilon_0 \frac{\partial E_{zy}}{\partial t} + \sigma_y E_{zy} &= -\frac{\partial H_x}{\partial y} \quad \text{(33b)} \\
\mu_0 \frac{\partial H_x}{\partial t} + \sigma^* H_x &= -\frac{\partial (E_{zx} + E_{zy})}{\partial y} \quad \text{(33c)} \\
\mu_0 \frac{\partial H_y}{\partial t} + \sigma^*_x H_y &= \frac{\partial (E_{zx} + E_{zy})}{\partial x} \quad \text{(33d)}
\end{align*}$$

The field components inside $\Gamma$ are $H_x, H_y, E_x$. The field components outside $\Gamma$ are $H_x, H_y, E_{zx}$ and $E_{zy}$. The field components on $\partial \Gamma$ are $H_x$ and $H_y$. The magnetic field is replaced with normalized version ($H = \sqrt{\frac{\mu_0}{\epsilon_0}} H$). The conductivity $\sigma$ is replaced with a normalized version ($\sigma \leftarrow \frac{\Lambda \sigma}{\epsilon_0}$).
The discrete form of the above equations is:

\[
(1 + \sigma_x)E_{xx}^{t+1}(i, j) = (1 - \sigma_x)E_{xx}^t(i, j) + \gamma \left[H_{xx}^{t+1/2}(i + 1/2, j) - H_{xx}^{t-1/2}(i - 1/2, j)\right]
\]

(34a)

\[
(1 + \sigma_y)E_{xy}^{t+1}(i, j) = (1 - \sigma_y)E_{xy}^t(i, j) - \gamma \left[H_{xy}^{t+1/2}(i, j + 1/2) - H_{xy}^{t-1/2}(i, j - 1/2)\right]
\]

(34b)

\[
(1 + \sigma_y^*)H_{xx}^{t+1/2}(i, j + 1/2) = (1 - \sigma_y^*)H_{xx}^{t-1/2}(i, j + 1/2) - \gamma \left[E_{xx}^{t}(i, j + 1) - E_{xx}^{t}(i, j) + E_{xy}^{t}(i, j + 1) - E_{xy}^{t}(i, j)\right]
\]

(34c)

\[
(1 + \sigma_x^*)H_{xy}^{t+1/2}(i + 1/2, j) = (1 - \sigma_x^*)H_{xy}^{t-1/2}(i + 1/2, j) + \gamma \left[E_{xx}^{t}(i + 1, j) - E_{xx}^{t}(i, j) + E_{xy}^{t}(i + 1, j) - E_{xy}^{t}(i, j)\right]
\]

(34d)

In order to get an impedance matching we need: \( \sigma_x = \sigma_x^* \) and \( \sigma_y = \sigma_y^* \). The profile of \( \sigma \) is \( \sigma(l) = \sigma_{\text{max}}(l/L)^2 \), were \( l \) is the layer index (\( l = 0 \ldots L - 1 \)), \( L \) is the total number of layers and \( \sigma_{\text{max}} \) is a tuning parameter.

Assuming \( L \) PML layers, Eqns. (34) involve \( 5 \cdot M \cdot L \) multiply-add operation in addition to the regular FDTD operations. The computational complexity of the PML will be equal to that of the GFM if \( 5 \cdot M \cdot L = M \cdot N^2 \), i.e., if \( N = \sqrt{5 \cdot L} \). For example, \( L = 20 \) layers of PML require the same computational resources as \( N = 10 \) terms in the Green’s function.

III.C.2 Stability

As presented in [19], the GFM in the two and three dimensions cases is potentially unstable. By modifying the simulation parameters (i.e., \( \gamma \) or \( N \)), a stabilized algorithm may be reached. Other methods of stabilization are also presented in [19].

In comparison, the Mur method is known to be stable for the two-dimensional case. The PML method, though, may become unstable when applied over an unbounded period of time. However, like the GFM, this potential source of problems is of little practical importance.

III.C.3 Accuracy and flexibility

In order to test the accuracy of the GFM, the aperture problem was used (Section III.B.4). A reference problem was first created by embedding the basic structure in a relatively large \((400 \times 400)\) grid, such that no reflections would arise within the first 100 timesteps. The results of the GFM agree with the reference solution with a total return loss of \(-26\) dB. As in the former examples, this figure should be interpreted in the comparative sense only, relative to the Mur and PML methods. The latter yield reflection errors of \(-8.8\) dB and \(-30\) dB, respectively, in this case. The PML case
was implemented with \( L = 5 \) layers in order to maintain equal number of *equivalent layers* (see discussion in Section III.C.1), and a parabolic profile \( (\sigma = \sigma_{\text{max}} \left( \frac{\Delta x}{N} \right)^2) \). Again, one can see that the GFM outperforms the Mur method, and is close to the performance of the PML. The results show that the accuracy of the GFM exceeds that of the Mur method and approaches that of the PML method. It should kept in mind, however, that the GFM has the unique capability of treating arbitrarily shaped media, such as the one shown in Section III.B.3 above.

### III.C.4 Summary

Results and conclusions from the three 2-D examples shown above, for the GFM, Mur and PML methods, are summarized in Table 3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>GFM ((N = 5))</th>
<th>Mur - First Order</th>
<th>PML ((L = 5))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical</td>
<td>( \propto M \cdot N^2 )</td>
<td>( \propto M )</td>
<td>( \propto 5 \cdot M \cdot L )</td>
</tr>
<tr>
<td>complexity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stability</td>
<td>potentially unstable</td>
<td>stable</td>
<td>potentially unstable</td>
</tr>
<tr>
<td>Reflection error</td>
<td>-32 dB</td>
<td>-22 dB</td>
<td>-38 dB</td>
</tr>
<tr>
<td>Programming</td>
<td>fair</td>
<td>low</td>
<td>high</td>
</tr>
<tr>
<td>complexity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Geometric</td>
<td>good</td>
<td>poor</td>
<td>poor</td>
</tr>
<tr>
<td>Adativity</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\( M = \text{Number of boundary points.} \)
\( N = \text{Order of the GFM approximation.} \)
\( L = \text{Number of layers.} \)

Table 3: Typical performance figures compared between the 2-D GFM, First Order Mur and PML methods, with \( L = N = 5 \). Reflection errors are valid in the comparative sense only.
IV Three Dimensional Case

IV.A Algorithm Description

Proceeding now to a three dimensional case, we make use of the 3-D Yee grid, whereby the following equations apply:

\[
\begin{align*}
H_x^{n+1} &= H_x^n + \gamma \left[ E_y^{n+\frac{1}{2}}(z^+) - E_y^{n+\frac{1}{2}}(z^-) - E_z^{n+\frac{1}{2}}(y^+) + E_z^{n+\frac{1}{2}}(y^-) \right] & (35a) \\
H_y^{n+1} &= H_y^n + \gamma \left[ E_z^{n+\frac{1}{2}}(x^+) - E_z^{n+\frac{1}{2}}(x^-) - E_x^{n+\frac{1}{2}}(z^+) + E_x^{n+\frac{1}{2}}(z^-) \right] & (35b) \\
H_z^{n+1} &= H_z^n + \gamma \left[ E_x^{n+\frac{1}{2}}(y^+) - E_x^{n+\frac{1}{2}}(y^-) - E_y^{n+\frac{1}{2}}(x^+) + E_y^{n+\frac{1}{2}}(x^-) \right] & (35c) \\
E_x^{n+\frac{1}{2}} &= E_x^n - \frac{1}{2} \gamma \left[ H_z^n(y^+) - H_z^n(y^-) - H_y^n(z^+) + H_y^n(z^-) \right] & (35d) \\
E_y^{n+\frac{1}{2}} &= E_y^n - \frac{1}{2} \gamma \left[ H_x^n(z^+) - H_x^n(z^-) - H_z^n(x^+) + H_z^n(x^-) \right] & (35e) \\
E_z^{n+\frac{1}{2}} &= E_z^n - \frac{1}{2} \gamma \left[ H_y^n(x^+) - H_y^n(x^-) - H_x^n(y^+) + H_x^n(y^-) \right] & (35f)
\end{align*}
\]

The examples worked out herein pertain to a rectangular waveguide, where the boundary is a plane \(z = z_{\text{max}}\) which is subject to many angles of incidence due to its excitation by an arbitrary mode. These examples are used to verify the ability of the GFM to represent arbitrary 3-D media beyond the boundary. To this end, we demonstrate two cases: (a) A waveguide with a matched load (i.e., an infinite waveguide), and (b) a waveguide with an obstacle beyond the boundary. Care is given in these cases for the choice of the boundary plane \(z = z_{\text{max}}\), in order to economize on algebraic operations. This is done by selecting a plane with a minimal number of field components when a specific field type (i.e., TE or TM) can be isolated.

IV.B Infinite Rectangular Waveguide Examples - with and without a conducting post

We begin with a simple example of an infinite rectangular waveguide, such that no physical reflections should be present. The geometry is shown in Fig. 17. The waveguide has a cross section of 21 \(\Delta x \times 11 \cdot \Delta y\) and is 301 \(\Delta z\) long. We define \(\Gamma\) as the area bounded by the planes \(z = \Delta z\) and \(z = 35\Delta z\). A TE\(_{10}\) mode is excited by the setting the boundary condition at \((z = \Delta z)\) as the appropriate distribution of \(E_y\). In order to apply the GFM boundary condition at \(\partial \Gamma : z = 35\Delta z\), we first generate the Green’s matrix describing the impulse responses of the tangential field components \(E_x\) and \(E_y\) over \(\partial \Gamma\). FDTD simulations with the GFM as the boundary condition are depicted in Figs. 18a and 18b, where the \(E_y\) field is shown along the X and Y axes, respectively,
after 95 timesteps. From these figures it can be seen that the sinusoidal mode profile in the X and Z directions, and the constant profile along the Y direction, are reconstructed quite accurately (relative error of \(-24\) dB for \(N = 6\) and \(\gamma = 0.3\)).

In the next example, the region \(\Gamma\) is made to be quite complex. It includes a conducting post as shown in Fig. 17, hence the Green’s function at \(z = z_{\text{max}}\) should include the effects of the post. Note that the post is lower than the height of the waveguide, which will cause the generation all modes of the type \(\text{TE}_{nm}\) when the waveguide is excited with the \(\text{TE}_{10}\) mode. The FDTD computation using the GFM Green’s matrix representing the complex medium \(\Gamma\), yields a solution which is compared against a reference simulation with an extended computational domain which includes the post. In this case all three field components, located at the boundary, \((\text{e.g., } E_x, E_y \text{ and } H_z)\) must be included in the calculation of the Green’s function and the FDTD simulation. The GFM computation has been performed with varying temporal durations. As expected, the longer the temporal duration the more accurate the results are. The reference solution is shown in Fig. 19a, where the electric field \(E_y\) is plotted along the \(X\)-axis (also depicted as the \(ABCD\) plane in Fig. 17). The effect of the conducting post is clearly seen as a region of null field. The FDTD results using the GFM are shown in Fig. 19b. This figure covers the region of \(\Gamma\) only, replacing the complementary region with a null field. In \(\Gamma\), the profiles of the two figures are the same. A more detailed comparison is presented in Fig. 20 where the reference and GFM-generated electrical fields along the center of the waveguide \((E - F \text{ line})\) are plotted. These two solutions are nearly identical within \(\Gamma\). For a Green’s function with \(N = 20\), the error along \(E - F\) line was \(-43\) dB after 150 timesteps. This error is further reduced to the level of \(-60\) dB using \(N = 60\). It should be noted that no comparison is made with either the Mur or PML methods, because the treatment of a complex medium beyond the boundary, as shown here, is considered a unique feature of the GFM.

V Conclusions

The GFM possesses three unique properties, i.e., accommodation of (1) arbitrarily shaped boundaries, in close proximity to the scattering object and (2) arbitrary composition of the exterior of the simulation space, coupled with (3) the simplicity of its application, which requires no problem-dependent tuning except for a suitable choices of \(\gamma\) and \(N\). The first property makes it possible to significantly reduce the size of the “white space” which otherwise would be required to conform, say, to a rectangular box. The second property allows one to specify a minimal computational domain, yet include the physical effects that occur outside of it. Moreover, it allows for the computation
of various configurations within the computational space given a fixed exterior. It should be noted that physical reflections from the exterior domain, when present, will be maintained naturally in the form of longer vectors representing the Green's function, in accordance with the actual time needed for the reflections to die out. One might also envision a generalization of the GFM which will characterize finite regions, rather than external regions, by suitable Green's functions. These Green's functions, however, need to be generated in the way described in Section II.A, i.e., by exciting the specified region by an impulse on the boundary, using Dirichlet boundary conditions. The concave boundary may then give rise to multiple reflections within the regions. This artifact will create long Green's function vectors, which do not represent physical reality and will hamper efficiency and accuracy. A more realistic extension will involve the treatment of Reentrant, or concave boundaries, which might still introduce longer vectors. These cases are treated in [19], with very good results. In terms of accuracy, the GFM results have been shown to be of a similar quality to the PML, and decidedly superior to the Mur condition. The GFM Green's function is formulated in a manner which naturally incorporates numerically induced effects, such as the numerical dispersion associated with the FDTD scheme. When $M, N \rightarrow \infty$, the GFM becomes an ideal absorber in the discretized space. This property should be contrasted to other methods which are initially designed for the continuum and are subsequently discretized, thereby incurring inherent errors in the discrete space which can not be eliminated unless the continuous limit is recovered.

The properties mentioned herein have been substantiated by a number of numerical examples, as described in this paper.

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