Efficiency of the Perfectly Matched Layer with High-Order Finite Difference and Pseudo-Spectral Maxwell Solvers

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Abstract

The commonly used second order Finite-Difference Time-Domain (FDTD) scheme for electromagnetic solvers in Particle-In-Cell codes produces fast solvers that scale well in parallel, but suffers from anomalous numerical effects resulting from discretization, such as numerical dispersion. High order schemes are therefore seen as the remedy for reducing the discretization errors. In the modeling of various applications, an open boundary is necessary for simulating vacuum extending beyond the computational box, for which algorithms based on - or derived from - Bérenger's Perfectly Matched Layers (PML) have demonstrated high efficiency over a wide range of wavelength and angle of incidence. The amount of numerical reflection of PMLs has been studied numerically and analytically for low order stencils but not systematically at higher order, nor for the pseudo-spectral scheme. In this paper, we extend the theoretical and numerical analysis of the coefficient of reflection of PML layers to solvers of any order of accuracy. Results show that the PML efficiency is preserved at any order, including at the infinite order limit that is attained by the pseudo-spectral formulation.

Keywords: Perfectly Matched (PML), High Order FDTD, Pseudo-Spectral Solvers

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1. Introduction

Particle-in-cell (PIC) has been the method of choice for the last fifty years for modeling plasmas that include kinetic effects. The most popular electromagnetic formulation uses second-order finite difference discretization of Maxwell's equations in both space and time (FDTD) which produces fast solvers that scale well in parallel, but suffers from various anomalous numerical effects resulting from discretization, such as numerical dispersion. High-order schemes [1] reduce the discretization errors at the expense of a computational cost that rises with the order of accuracy. Beyond a certain order which depends on the details of implementation and the hardware used for the simulations, it is well known that pseudo-spectral methods become eventually more efficient than finite-difference methods [2].

In 1973, Haber et al. presented a pseudo-spectral solver that integrates analytically the solution over a finite time step, under the assumption that the source is constant over that time step [3]. Haber's pseudo-spectral analytical time-domain (PSATD) particle in cell (PIC) algorithm has various advantages over the FDTD as it solves the vacuum Maxwell's equations exactly, has no Courant time-step limit, offers substantial flexibility in plasma and particle beam simulations is more stable with regard to Numerical Cerenkov [4]. The other commonly used pseudo-spectral time-domain (PSTD) algorithm offers similar advantages except for a restrictive Courant limit.

However the difficulty for efficient parallelization owing to global communications associated with global FFTs on the entire computational domains has rendered the pseudo-spectral solvers rarely used in PIC simulations. Recently, a new method was proposed for the parallelization of electromagnetic pseudo-spectral solvers, offering the potential for solvers combining the favorable parallel scaling of standard FDTD with the accuracy of pseudo-spectral methods [5].

In many cases, an open boundary condition is required on one or more boundary of the simulation box. In these cases, various techniques have been used such as the one way approximation of the wave equation (initially exhibited for acoustic waves) by Engquist and Majda [6], or Bérenger's more efficient Perfectly Matched Layer (PML) technique which consists in surrounding the computational domain with an absorbing medium whose impedance matches that of free-space. While a PML medium absorbs waves at all wavelength and angle of incidence at the infinitesimal limit, spurious reflections occur due to discretization. The amount of reflection as a func-

tion of wavelength and angle of incidence has been evaluated numerically and analytically at low order discretization [7] but not systematically at higher order. While an implementation of the PML in a PSTD solver was given by Ohmura et al. [8], the estimates of the coefficients of reflection with respect to wavelength and angle were not given. The analysis carried out in this article focuses on Bérenger's split field original formulation Maxwell's equations of PML medium, as it is the implementation that is currently used in the targeted plasma simulation code. Application to other PML formulation, such as complex coordinate stretching [9, 10] is left for future work.

The exponential convergence of the PML solution to the unbounded domain has been demonstrated in previous work [11] at the infinitesimal limit. This, however, does not guarantee high absorption rates at any angle and frequency with the discretized form of the PML. In particular, since the PML condition is local, it is nonetheless necessary to study carefully its efficiency when used with high-order stencils, when the extent of the stencil can exceed the PML thickness, and especially with pseudo-spectral algorithms that involve global FFT operations. In this study, we extend the theoretical and numerical analysis of the coefficient of reflection of PML to solvers of any order of accuracy, taking the limit of infinite order to obtain the solutions for the pseudo-spectral formulations.

2. The Perfectly Matched Layer (PML) in high-order and pseudo-spectral solvers

2.1. Definition of the PML Medium

2.1.1. Formulation of the PML Medium

In this paper, we consider, for simplicity and without loss of generality, the TE (transverse electric) mode, which involves in Cartesian coordinates the field components E_x , E_y and B_z .

A PML medium involves an electric conductivity σ and a magnetic conductivity σ^* , with a split of the Maxwell's equations, and writes as follows

for the TE mode [12]:

$$\frac{\partial E_x}{\partial t} + \sigma_y E_x = c^2 \frac{\partial B_z}{\partial y}, \quad (2.1)$$

$$\frac{\partial E_y}{\partial t} + \sigma_x E_y = -c^2 \frac{\partial B_z}{\partial x}, \quad (2.2)$$

$$\frac{\partial B_{zx}}{\partial t} + \sigma_x^* B_{zx} = -\frac{\partial E_y}{\partial x}, \quad (2.3)$$

$$\frac{\partial B_{zy}}{\partial t} + \sigma_y^* B_{zy} = \frac{\partial E_x}{\partial y}, \quad (2.4)$$

with c the speed of light, $\partial/\partial t$ partial differential in time, $\partial/\partial x$ and $\partial/\partial y$ partial differentials respectively in x - and y -directions, and $B_z = B_{zx} + B_{zy}$. This medium absorbs electromagnetic waves at any wavelength and angle of incidence if its impedance matches the one of vacuum, which happens when $\sigma_x/\epsilon_0 = \sigma_x^*/\mu_0$ and $\sigma_y/\epsilon_0 = \sigma_y^*/\mu_0$ (also known as the matching conditions) [12].

2.2. Discretization of the PML

The FDTD discretization (second order on a staggered mesh in space and in time) of equations (2.1-2.4) is given by

$$\begin{aligned} \frac{E_{i+1/2,j}^{n+1} - E_{i+1/2,j}^n}{\Delta t} + \sigma_y \frac{E_{i+1/2,j}^{n+1} + E_{i+1/2,j}^n}{2} &= c^2 \frac{B_{i+1/2,j+1/2}^{n+1/2} - B_{i+1/2,j-1/2}^{n+1/2}}{\Delta y}, \\ \frac{E_{i,j+1/2}^{n+1} - E_{i,j+1/2}^n}{\Delta t} + \sigma_x \frac{E_{i,j+1/2}^{n+1} + E_{i,j+1/2}^n}{2} &= -c^2 \frac{B_{i+1/2,j+1/2}^{n+1/2} - B_{i-1/2,j+1/2}^{n+1/2}}{\Delta x}, \\ \frac{B_{zx,i+1/2,j+1/2}^{n+1/2} - B_{zx,i+1/2,j+1/2}^{n-1/2}}{\Delta t} + \sigma_x^* \frac{B_{zx,i+1/2,j+1/2}^{n+1/2} + B_{zx,i+1/2,j+1/2}^{n-1/2}}{2} &= -\frac{E_{i+1,j+1/2}^n - E_{i,j+1/2}^n}{\Delta x}, \\ \frac{B_{zy,i+1/2,j+1/2}^{n+1/2} - B_{zy,i+1/2,j+1/2}^{n-1/2}}{\Delta t} + \sigma_y^* \frac{B_{zy,i+1/2,j+1/2}^{n+1/2} + B_{zy,i+1/2,j+1/2}^{n-1/2}}{2} &= \frac{E_{i+1/2,j+1}^n - E_{i+1/2,j}^n}{\Delta y}. \end{aligned} \quad (2.5)$$

After some algebraic manipulation, equations in (2.5) can be written in their explicit linear forms for implementation in a simulation code

$$\begin{aligned} E_{i+1/2,j}^{n+1} &= \alpha_x E_{i+1/2,j}^n + \beta_x \left(B_{i+1/2,j+1/2}^{n+1/2} - B_{i+1/2,j-1/2}^{n+1/2} \right), \\ E_{i,j+1/2}^{n+1} &= \alpha_y E_{i,j+1/2}^n + \beta_y \left(B_{i+1/2,j+1/2}^{n+1/2} - B_{i-1/2,j+1/2}^{n+1/2} \right), \\ B_{zx,i+1/2,j+1/2}^{n+1/2} &= \alpha_x^* B_{zx,i+1/2,j+1/2}^{n-1/2} + \beta_x^* \left(E_{i+1,j+1/2}^n - E_{i,j+1/2}^n \right), \\ B_{zy,i+1/2,j+1/2}^{n+1/2} &= \alpha_y^* B_{zy,i+1/2,j+1/2}^{n-1/2} + \beta_y^* \left(E_{i+1/2,j+1}^n - E_{i+1/2,j}^n \right). \end{aligned} \quad (2.6)$$

where

$$\begin{cases} \alpha_x = \frac{2-\sigma_y \Delta t}{2+\sigma_y \Delta t}, \\ \alpha_y = \frac{2-\sigma_x \Delta t}{2+\sigma_x \Delta t}, \\ \beta_x = \frac{2c^2}{2+\sigma_y \Delta t} \frac{\Delta t}{\Delta y}, \\ \beta_y = -\frac{2c^2}{2+\sigma_x \Delta t} \frac{\Delta t}{\Delta x}, \\ \alpha_x^* = \frac{2-\sigma_x^* \Delta t}{2+\sigma_x^* \Delta t}, \\ \alpha_y^* = \frac{2-\sigma_y^* \Delta t}{2+\sigma_y^* \Delta t}, \\ \beta_x^* = -\frac{2}{2+\sigma_x^* \Delta t} \frac{\Delta t}{\Delta x}, \\ \beta_y^* = \frac{2}{2+\sigma_y^* \Delta t} \frac{\Delta t}{\Delta y}. \end{cases} \quad (2.7)$$

2.3. Extension to Higher Order

The extension to order N in the space domain of the explicit linear form can be written as the following general expression

$$\begin{aligned} E_i^{n+1} &= \alpha E_i^n + \beta \left[C_1 \left(B_{i+1/2}^{n+1/2} - B_{i-1/2}^{n+1/2} \right) + C_2 \left(B_{i+3/2}^{n+1/2} - B_{i-3/2}^{n+1/2} \right) + \dots \right] \\ &= \alpha E_i^n + \beta \sum_{m=1}^N C_m \left(B_{i+(2m-1)/2}^{n+1/2} - B_{i-(2m-1)/2}^{n+1/2} \right), \end{aligned} \quad (2.8)$$

where α, β are constants (refer to 2.7) and C_m are the coefficients of finite-difference approximation [1]. For this study, we use the coefficients given by an algorithm due to Fornberg [13], which are given in Table 1 for orders 2 to 20, and at the limit of infinite order, and apply to equispaced staggered grids [13].

Order of accuracy	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	position= $\frac{11}{2}$	$\frac{13}{2}$	$\frac{15}{2}$	$\frac{17}{2}$	$\frac{19}{2}$
2	1.0000									
4	1.1250	-.0417								
6	1.1719	-.0651	.0047							
8	1.1963	-.0798	.0096	-7.0e(-4)						
10	1.2112	-.0897	.0138	-1.8e(-3)	1.2e(-4)					
12	1.2213	-.0969	.0174	-3.0e(-3)	3.6e(-4)	-2.2e(-5)				
14	1.2286	-.1024	.0205	-4.2e(-3)	6.9e(-4)	-7.7e(-5)	4.2e(-6)			
16	1.2341	-.1066	.0230	-5.3e(-3)	1.1e(-3)	-1.6e(-4)	1.7e(-5)	-8.5e(-7)		
18	1.2384	-.1101	.0252	-6.4e(-3)	1.5e(-3)	-2.9e(-4)	4.1e(-5)	-3.8e(-6)	1.8e(-7)	
20	1.2418	-.1129	.0271	-7.4e(-3)	1.9e(-3)	-4.3e(-4)	7.7e(-5)	-1.0e(-5)	8.8e(-7)	-3.7e(-8)
⋮										
limit $N \rightarrow \infty$	1.2732	-.1415	.0509	-.0260	.0157	-.0105	.0075	-.0057	.0044	-.0035

Table 1: Coefficients of discretization generated from Fornberg's algorithm

A similar expression applies to $B_{i+1/2}^{n+1/2}$, written as

$$B_{i+1/2}^{n+1/2} = \alpha^* B_{i+1/2}^{n-1/2} + \beta^* \sum_{m=1}^N C_m \left(E_{y_{i+m}}^{n+1/2} - E_{y_{i-(m-1)}}^{n+1/2} \right). \quad (2.9)$$

2.4. Application to Staggered-Grid Pseudo-Spectral Time-Domain (PSTD) Solvers

In the PSTD implementation, the Fourier transformation is used for the calculation of the spatial differentiation in k-space, while the Leapfrog method is retained for the temporal differentiation. Following the notations given in [8] the PSTD formulation of the set of equations (2.1-2.4) is given by:

$$\frac{\partial E_x}{\partial t} + \sigma_y E_x = c^2 [\mathcal{F}^{-1} i k_y (\mathcal{F} B_z)], \quad (2.10)$$

$$\frac{\partial E_y}{\partial t} + \sigma_x E_y = -c^2 [\mathcal{F}^{-1} i k_x (\mathcal{F} B_z)], \quad (2.11)$$

$$\frac{\partial B_{zx}}{\partial t} + \sigma_x^* B_{zx} = -[\mathcal{F}^{-1} i k_x (\mathcal{F} E_y)], \quad (2.12)$$

$$\frac{\partial B_{zy}}{\partial t} + \sigma_y^* B_{zy} = [\mathcal{F}^{-1} i k_y (\mathcal{F} E_x)]. \quad (2.13)$$

Assuming the use of a staggered grid (Yee discretization), the discretized form can be written as follows

$$\begin{aligned} \frac{E_{x_{i+1/2,j}}^{n+1} - E_{x_{i+1/2,j}}^n}{\Delta t} + \sigma_y \frac{E_{x_{i+1/2,j}}^{n+1} + E_{x_{i+1/2,j}}^n}{2} &= c^2 \left[\mathcal{F}^{-1} i k_y e^{-i k_y \Delta y/2} \left(\mathcal{F} B_{z_{i+1/2,j}}^{n+1/2} \right) \right], \\ \frac{E_{y_{i,j+1/2}}^{n+1} - E_{y_{i,j+1/2}}^n}{\Delta t} + \sigma_x \frac{E_{y_{i,j+1/2}}^{n+1} + E_{y_{i,j+1/2}}^n}{2} &= -c^2 \left[\mathcal{F}^{-1} i k_x e^{-i k_x \Delta x/2} \left(\mathcal{F} B_{z_{i,j+1/2}}^{n+1/2} \right) \right], \\ \frac{B_{zx_{i+1/2,j+1/2}}^{n+1/2} - B_{zx_{i+1/2,j+1/2}}^{n-1/2}}{\Delta t} + \sigma_x^* \frac{B_{zx_{i+1/2,j+1/2}}^{n+1/2} + B_{zx_{i+1/2,j+1/2}}^{n-1/2}}{2} &= -[\mathcal{F}^{-1} i k_x e^{i k_x \Delta x/2} (\mathcal{F} E_{y_{i+1/2,j+1/2}}^n)], \\ \frac{B_{zy_{i+1/2,j+1/2}}^{n+1/2} - B_{zy_{i+1/2,j+1/2}}^{n-1/2}}{\Delta t} + \sigma_y^* \frac{B_{zy_{i+1/2,j+1/2}}^{n+1/2} + B_{zy_{i+1/2,j+1/2}}^{n-1/2}}{2} &= [\mathcal{F}^{-1} i k_y e^{i k_y \Delta y/2} (\mathcal{F} E_{x_{i+1/2,j+1/2}}^n)]. \end{aligned} \quad (2.14)$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are respectively the forward and inverse Fourier transformations, k_x and k_y are the wavenumbers in the x - and y -directions. The terms $e^{i k_x \Delta x/2}$ and $e^{i k_y \Delta y/2}$ are respectively the shifts in space in x - and y -directions on the staggered grid for E_y , while the terms $e^{-i k_x \Delta x/2}$ and $e^{-i k_y \Delta y/2}$ are respectively the shifts in space in x - and y -directions on the staggered grid for B_z .

After some algebraic manipulation, the set of equations (2.14) is rewritten in its explicit linear form, giving

$$\begin{aligned}
\text{Ex}_{i+1/2,j}^{n+1} &= \alpha_x \text{Ex}_{i+1/2,j}^n + \beta_x \left[\mathcal{F}^{-1} i k_y e^{-i k_y \Delta y / 2} \left(\mathcal{F} \text{Bz}_{i+1/2,j}^{n+1/2} \right) \right], \\
\text{Ey}_{i,j+1/2}^{n+1} &= \alpha_y \text{Ey}_{i,j+1/2}^n + \beta_y \left[\mathcal{F}^{-1} i k_x e^{-i k_x \Delta x / 2} \left(\mathcal{F} \text{Bz}_{i,j+1/2}^{n+1/2} \right) \right], \\
\text{Bzx}_{i+1/2,j+1/2}^{n+1/2} &= \alpha_x^* \text{Bzx}_{i+1/2,j+1/2}^{n-1/2} + \beta_x^* \left[\mathcal{F}^{-1} i k_x e^{i k_x \Delta x / 2} \left(\mathcal{F} \text{Ey}_{i+1/2,j+1/2}^n \right) \right], \\
\text{Bzy}_{i+1/2,j+1/2}^{n+1/2} &= \alpha_y^* \text{Bzy}_{i+1/2,j+1/2}^{n-1/2} + \beta_y^* \left[\mathcal{F}^{-1} i k_y e^{i k_y \Delta y / 2} \left(\mathcal{F} \text{Ex}_{i+1/2,j+1/2}^n \right) \right].
\end{aligned}$$

The coefficients of $(\alpha_x, \beta_x, \alpha_y, \beta_y, \alpha_x^*, \beta_x^*, \alpha_y^*, \beta_y^*)$ are the same as shown in 2.7.

3. Reflection of a Plane Wave Striking a PML

Following [7], the coefficient of reflection of a plane wave propagating in the x -direction perpendicularly to the interface of the PML can be computed with some analogy to the interferometer of Fabry-Perot by integrating over the multiple transmissions t and reflections r of rays between two rows of the grid (two plates in the interferometer).

Calculating the coefficient of reflection for the entire layer, denoted R , requires knowledge of the coefficients of reflection at each plane of the layer (nodes $i, i + 1/2, i + 1, \dots$), denoted r .

3.1. Coefficients of Reflection at Individual Planes

We begin by evaluating the coefficient of reflection at a row passing through a node situated at one of the slices in the PML media. The rest of the space is described by centered finite difference of the wave equation in vacuum. We assume that only the plane where the PML scheme applies generates reflections.

The basic procedure for the derivation of the coefficient of reflection involves substitution of plane monochromatic traveling-wave trial solutions into an expression that consists of only the components of a particular field. For instance, in the derivation of the coefficient of reflection on the full-node, we would like to obtain an expression consisting of only components of the field, Ey , implying that all components of Bz have to be eliminated. Hence, the method consists of deriving the finite difference expression for the second

derivative in time of E_y and then eliminate B_z by substituting the finite difference expression for the first time derivative of B_z in two adjacent nodes. It is instructive to follow the details of the derivation, therefore a walk-through is given in the following paragraphs.

3.1.1. One-dimensional case

Firstly, we express the finite difference expression for the second derivative in time of E_y , given by

$$E_y^{n+1} = \alpha_y E_y^n + \beta_y \sum_{m=1}^N C_m \left(B_z^{n+1/2}_{i+(2m-1)/2} - B_z^{n+1/2}_{i-(2m-1)/2} \right), \quad (3.1)$$

$$E_y^n = \alpha_y E_y^{n-1} + \beta_y \sum_{m=1}^N C_m \left(B_z^{n-1/2}_{i+(2m-1)/2} - B_z^{n-1/2}_{i-(2m-1)/2} \right), \quad (3.2)$$

where $N \in \mathbb{N}$.

Subtracting 3.2 from 3.1 then gives

$$\begin{aligned} E_y^{n+1} - E_y^n &= \alpha_y (E_y^n - E_y^{n-1}) \\ &\quad + \beta_y \sum_{m=1}^N C_m \left(B_z^{n+1/2}_{i+(2m-1)/2} - B_z^{n-1/2}_{i+(2m-1)/2} - B_z^{n+1/2}_{i-(2m-1)/2} + B_z^{n-1/2}_{i-(2m-1)/2} \right). \end{aligned} \quad (3.3)$$

On the other hand, we also have

$$B_z^{n+1/2}_{i+1/2} = B_z^{n-1/2}_{i+1/2} + V \sum_{m=1}^N C_m (E_y^n_{i+m} - E_y^n_{i-(m-1)}), \quad (3.4)$$

$$B_z^{n+1/2}_{i-1/2} = B_z^{n-1/2}_{i-1/2} + V \sum_{m=1}^N C_m (E_y^n_{i+m-1} - E_y^n_{i-m}), \quad (3.5)$$

where $V = c^2 \Delta t / \Delta x$.

The eliminates of B_z is obtained by insertions of equations 3.4 and 3.5 in equation 3.3.

We now assume a plane monochromatic traveling-wave trial solution of amplitude $e^{i(\omega \Delta t - k \Delta x)}$ striking the PML slice at normal incidence. We also assume that the norm of k is conserved by the transmitted and the reflected waves and we define the coefficient of reflection as the complex number r .

Under these conditions, the transmitted wave is given by $(1 - r) e^{i(\omega\Delta t - k\Delta x)}$, and the signal in front of the slice is the sum of the incident wave and the reflected one, given by $e^{i(\omega\Delta t - k\Delta x)} - r e^{i(\omega\Delta t + k\Delta x)}$. Assuming that the PML is applied at the slice located at i , we have

$$E y_{i+N_x}^{n-N_t} = (1 - r) e^{-N_t i \omega \Delta t - N_x i k \Delta x}, \quad (3.6)$$

$$E y_{i+N_x}^{n+N_t} = (1 - r) e^{N_t i \omega \Delta t - N_x i k \Delta x}, \quad (3.7)$$

$$E y_{i-(N_x+1)}^{n-N_t} = e^{-N_t i \omega \Delta t + (N_x+1) i k \Delta x} - r e^{-N_t i \omega \Delta t - (N_x+1) i k \Delta x}, \quad (3.8)$$

$$E y_{i-(N_x+1)}^{n+N_t} = e^{N_t i \omega \Delta t + (N_x+1) i k \Delta x} - r e^{N_t i \omega \Delta t - (N_x+1) i k \Delta x}, \quad (3.9)$$

where $N_t \in \mathbb{N}$ and $N_x \in \mathbb{N}$.

By inserting the plane monochromatic traveling-wave trial solutions, we obtain, to leading order, the coefficient of reflection at a full-node

$$r_{node} = \frac{a - b \sum_{N=0}^{\infty} C_{coupled_N} \cos N k \Delta x}{a - b \sum_{N=0}^{\infty} C_{coupled_N} e^{-i N k \Delta x}}, \quad (3.10)$$

where

$$\begin{cases} a &= e^{i \omega \Delta t} - 1 - \alpha_y + \alpha_y e^{-i \omega \Delta t}, \\ b &= 2 \beta_y V. \end{cases}$$

$C_{coupled_N}$ are the coupled Fornberg's coefficients, defined by

$$C_{coupled_N} = \begin{cases} -\sum_{i=1}^{norder} C_i^2, & \text{if } N = 0, \\ -2 \sum_{i=1}^{norder} C_i C_{i-N}, & \text{if } 0 < N < norder, \\ 2 \sum_{i=1}^{norder} C_i C_{N-(i-1)}, & \text{if } norder \leq N < 2norder - 1, \\ \sum_{i=1}^{norder} C_i^2, & \text{if } N = 2norder - 1, \end{cases} \quad (3.11)$$

where $norder$ is the number of the order of discretization, and C are the coefficients from Fornberg's algorithm [13] (Table 1).

The derivation of the coefficient of reflection at an inter-node $r_{inter-node}$ (not detailed here) proceeds similarly and gives an expression of the same form as 3.10, after replacement of α_y by α_y^* and β_y by β_y^* in the definition of a and b .

3.1.2. Two-dimensional case

The derivation of the coefficient of reflection at higher dimension requires more algebraic manipulation. As in the previous section, the derivation of

the coefficient of reflection involves the substitution of plane monochromatic traveling-wave trial solutions into an expression that consists of only the components of a particular field.

The equations to be solved at a node are given by

$$\text{Ey}_{i,j+1/2}^{n+1} = \alpha_y \text{Ey}_{i,j+1/2}^n - \beta_y \sum_{m=1}^N C_m \left(\text{Bz}_{i+(2m-1)/2,j+1/2}^{n+1/2} - \text{Bz}_{i-(2m-1)/2,j+1/2}^{n+1/2} \right), \quad (3.12)$$

$$\begin{aligned} \text{Ey}_{i+1,j+1/2}^n &= \text{Ey}_{i,j+1/2}^n + \frac{\Delta x}{\Delta y} (\text{Ex}_{i+1/2,j+1}^n - \text{Ex}_{i+1/2,j}^n) \\ &\quad - \frac{\Delta x}{\Delta t} \left(\text{Bz}_{i+1/2,j+1/2}^{n+1/2} - \text{Bz}_{i+1/2,j+1/2}^{n-1/2} \right), \end{aligned} \quad (3.13)$$

$$\text{Ex}_{i+1/2,j+1}^n = \text{Ex}_{i+1/2,j+1}^{n-1} + V_y \sum_{m=1}^N C_m \left(\text{Bz}_{i+1/2,j+(2m+1)/2}^{n+1/2} - \text{Bz}_{i+1/2,j-(2m-3)/2}^{n+1/2} \right), \quad (3.14)$$

where $V_y = c^2 \Delta t / \Delta y$.

A different approach is applied to derive the coefficient of reflection on the inter-node, for which the following set of equations is solved

$$\text{Ex}_{i+1/2,j}^{n+1} = \text{Ex}_{i+1/2,j}^n + V_y \sum_{m=1}^N C_m \left(\text{Bz}_{i+1/2,j+(2m-1)/2}^{n+1/2} - \text{Bz}_{i+1/2,j-(2m-1)/2}^{n+1/2} \right) \quad (3.15)$$

$$\text{Ey}_{i,j+1/2}^{n+1} = \text{Ey}_{i,j+1/2}^n - V_x \sum_{m=1}^N C_m \left(\text{Bz}_{i+(2m-1)/2,j+1/2}^{n+1/2} - \text{Bz}_{i-(2m-1)/2,j+1/2}^{n+1/2} \right), \quad (3.16)$$

$$\text{Bz}_{i+1/2,j+1/2}^{n+1/2} = \text{Bzx}_{i+1/2,j+1/2}^{n+1/2} + \text{Bzy}_{i+1/2,j+1/2}^{n+1/2}, \quad (3.17)$$

$$\text{Bzx}_{i+1/2,j+1/2}^{n+1/2} = \alpha_x^* \text{Bzx}_{i+1/2,j+1/2}^{n-1/2} - \beta_x^* \sum_{m=1}^N C_m (\text{Ey}_{i+m,j+1/2}^n - \text{Ey}_{i-(m-1),j+1/2}^n), \quad (3.18)$$

$$\text{Bzy}_{i+1/2,j+1/2}^{n+1/2} = \text{Bzy}_{i+1/2,j+1/2}^{n-1/2} + \frac{\Delta t}{\Delta y} \sum_{m=1}^N C_m (\text{Ex}_{i+1/2,j+m}^n - \text{Ex}_{i+1/2,j-(m-1)}^n), \quad (3.19)$$

where $V_x = c^2 \Delta t / \Delta x$ and $V_y = c^2 \Delta t / \Delta y$.

Solving the systems of equations given above leads to the same form for the expression of the coefficient of reflection at the node and the inter-node, which reads (for a node):

$$r_{node} = \frac{a - b \sum_{N=0}^{\infty} C_{coupled_N} \cos N k_y \Delta y - c \sum_{N=0}^{\infty} C_{coupled_N} \cos N k_x \Delta x}{a - b \sum_{N=0}^{\infty} C_{coupled_N} \cos N k_y \Delta y - c \sum_{N=0}^{\infty} C_{coupled_N} e^{-i N k_x \Delta x}}, \quad (3.20)$$

where

$$\begin{cases} a &= e^{i\omega \Delta t} - (2 + \alpha_y) + e^{-i\omega \Delta t} (1 + 2\alpha_y) + \alpha_y e^{-2i\omega \Delta t}, \\ b &= 2V_y \frac{\Delta t}{\Delta y} (1 - \alpha_y e^{-i\omega \Delta t}), \\ c &= 2\beta_y \frac{\Delta t}{\Delta x} (1 - e^{-i\omega \Delta t}). \end{cases}$$

The coefficient of reflection on an inter-node, $r_{inter-node}$ is obtained by replacing α_y with α_x^* and β_y with β_x^* in the definition of a , b and c .

To guide the reader, the details of the derivation of these equations are given for the second order case in Appendices A and B, at the node and the inter-node respectively. A table summarizing the coefficients of reflections in various cases is given in Appendix C.

3.2. Coefficient of Reflection of the Entire PML, R

Figure 1: A plane wave striking a PML generates multiple reflections inside the layer that must be taken into account to calculate the coefficient of reflection.

Following [7], we apply the PML from j_0 to $j_0 + N_L$, where j_0 is the index where the interface of vacuum and the PML media lies and N_L is the depth of the PML (in number of nodes). The knowledge of the coefficients of reflection and transmission of two consecutive slices, say slices at $j_0 + N_L - 1/2$ and $j_0 + N_L$, allows us to calculate the coefficient of reflection $R_{j_0 + N_L - 1/2}$ resulting from the coupling of these two slices. Fig. 1 illustrates the reflections and transmissions of the wave of the two consecutive slices.

$$\begin{aligned} R_{j_0 + N_L - 1/2} &= r_1 - t_1 r_2 t_1 e^{-ik_x \Delta x} + t_1 r_2 t_1 e^{-ik_x \Delta x} (r_1 r_2 e^{-ik_x \Delta x}) \\ &\quad - t_1 r_2 t_1 e^{-ik_x \Delta x} (r_1 r_2 e^{-ik_x \Delta x})^2 \dots \\ &= r_1 - t_1 r_2 t_1 e^{-ik_x \Delta x} \sum_{n=0}^{\infty} (r_1 r_2 e^{-ik_x \Delta x})^n \\ &= r_1 - \frac{t_1 r_2 t_1 e^{-ik_x \Delta x}}{1 + r_1 r_2 e^{-ik_x \Delta x}}. \end{aligned} \quad (3.21)$$

The coefficient of reflection of the entire layer R_{j_0} is obtained by iterating backward from $j = j_0 + N_L$ to $j = j_0$ using the recursive formula

$$R_j = r_j - \frac{t_j R_{j+1/2} t_j e^{-ik_x \Delta x}}{1 + r_j R_{j+1/2} e^{-ik_x \Delta x}}. \quad (3.22)$$

This formula is valid at any dimension and, under the assumptions of the model, at any order.

3.3. Coefficient of Reflection via Numerical Simulations

For the evaluation of the coefficient of reflection via numerical experiments, an electromagnetic pulse is injected at $t = 0$ at the left-hand side of the simulation region, in a vacuum region preceding the PML that is situated at the right-hand side. Periodic boundaries are applied to the upper and lower sides. The simpler case of a plane wave at normal incidence to the PML media is studied first, followed by a study of a plane wave traveling at an angle of incidence to the PML.

The injected signal that is imposed at the left-hand side $Ey_0^0 = F(\omega, t, k_y)$ has the form

$$F(\omega, t, k_y) = \begin{cases} H(t) \sin(\omega t + k_y y), & \text{when } 0 < t < \frac{L}{c}, \\ 0, & \text{otherwise,} \end{cases} \quad (3.23)$$

with $y = j \Delta y$, where j is the index in the transverse (y) direction, and $H(t)$ is the Harris function

$$H(t) = \begin{cases} \frac{1}{32} (10 - 15 \cos(\frac{2\pi ct}{L}) + 6 \cos(\frac{4\pi ct}{L}) - \cos(\frac{6\pi ct}{L})), & \text{when } 0 < t < \frac{L}{c}, \\ 0, & \text{otherwise,} \end{cases} \quad (3.24)$$

where $L = N_x \Delta x$ is the distance separating the injection point to the PML, and c is the speed of light. A plot of this function versus time is reproduced in Fig. 2. The product of the $\sin(\omega t)$ function with the Harris function generates a quasi-monochromatic signal, as seen by its Fourier transform in Fig. 2, with a compact support, enabling a precise inspection of the coefficient of reflection as a function of frequency.

Figure 2: The Fourier transform of $F(\omega, t, k_y = 0)$ with respect to the wavenumber k shows that the signal is nearly monochromatic. Inset: Harris function $H(t)$ and $F(\omega, t, k_y = 0)$ plotted versus time normalized by L/c .

For a given set of wavenumbers k_x and k_y , the angular wavelength ω is calculated from the 2D high-order numerical dispersion equation (equation 3.25),

$$\left[\frac{1}{c\Delta t} \sin \left(\frac{\omega \Delta t}{2} \right) \right]^2 = \left[\frac{1}{\Delta x} \sum_{N=1}^{\infty} C_N \sin \left(\frac{(2N-1) k_x \Delta x}{2} \right) \right]^2 + \left[\frac{1}{\Delta y} \sum_{N=1}^{\infty} C_N \sin \left(\frac{(2N-1) k_y \Delta y}{2} \right) \right]^2, \quad (3.25)$$

where C_N are the coefficients from Fornberg's algorithm.

For convenience, for a signal injected with a wavenumber k_0 , the transverse wavenumber k_y is set for a grid with N_y cells, and periodic boundary condition in the transverse dimension, as $k_y = 2\pi N/(N_y \Delta y)$ where $N \in \mathbb{N}$. The longitudinal wavenumber is thus given by $k_x^2 = k_0^2 - k_y^2$ and the angle of incidence ϕ is defined as $\phi = \arctan(k_y/k_x)$.

Once the injected pulse fills the vacuum region preceding the PML, the electric and magnetic field components Ex_{inc} , Ey_{inc} and Bz_{inc} are recorded, while the reflected components Ex_{refl} , Ey_{refl} and Bz_{refl} are recorded after the incident pulse has been fully reflected by the PML layer. The coefficient of reflection is then computed as

$$R(\omega, \phi) = \sqrt{\frac{\sum_{i < N_x} \sum_{j < N_y} (Ex_{refl}^2 + Ey_{refl}^2 + c^2 Bz_{refl}^2)}{\sum_{i < N_x} \sum_{j < N_y} (Ex_{inc}^2 + Ey_{inc}^2 + c^2 Bz_{inc}^2)}}, \quad (3.26)$$

where i and j are respectively the grid indices in the longitudinal (x) and transverse (y) directions.

4. Results

In this section, we compare the coefficient of reflection from a PML for the FDTD solver (of order 2 to higher orders) and the PSTD solver, as a function of wavelengths and angles, in the case $\Delta x = \Delta y$. To ensure stability at any order, the time step was chosen to be $c\Delta t/\Delta x = 0.4$, which is slightly below the Courant condition of the PSTD solver when $\Delta x = \Delta y$. Following [12], we define

$$\sigma_i = \sigma_{max} \left(\frac{i\Delta x}{\delta} \right)^n,$$

with $i \in [0; N_L]$ where N_L is the depth of the PML (in number of nodes). The choice of N_L is based on the theoretical coefficient of reflection such that it is large enough, for a given profile of the conductivity, that the reflections that occur on the last cell are negligible. Setting $\sigma_{max} = 4/\Delta x$, $\delta = 5\Delta x$ and $n = 2$, together with $N_L=14$, lead to absorptions of the incident waves by orders of magnitude at any angle, for all wavelength $\lambda > \Delta x/4$. In defining σ^* , one must take into account the half a step in the space grid since E and B are staggered in space, therefore $\sigma^* = \sigma_{i+1/2}$.

Figure 3: Coefficient of reflection with respect to the normalized wavelengths of a plane wave striking a PML at normal incidence (lines: analytical integration; markers: numerical simulations), for different orders going from 2 to infinity ($\equiv$ pseudo-spectral).

Figure 4: Coefficient of reflection of a plane wave with respect to its angle of incidence with the PML, for $\lambda/\Delta x = 4$ (lines: analytical integration; markers: numerical simulations).

Figure 5: Coefficient of reflection of a plane wave with respect to its angle of incidence with the PML, for $\lambda/\Delta x = 8$ (lines: analytical integration; markers: numerical simulations).

Figure 6: Theoretical estimates of the coefficient of reflection with respect to angle of incidence for $\lambda/dx = 32$.

Figure 7: Theoretical estimates of the coefficient of reflection with respect to angle of incidence for $\lambda/dx = 1024$.

Fig. 3 presents the coefficient of reflection of a plane wave that is striking a PML at normal incidence, as a function of wavelength. Fig. 4 and 5 show the coefficient of reflection of a plane wave with respect to the angle of incidence for a given wavelength, while Fig. 6 and 7 show the theoretical estimates for larger wavelengths. The results show that the efficiency of the PML is preserved at any order and even improves at short wavelengths with higher orders. This is also verified by the PSTD solver for which, as expected, the coefficients of reflection are very close to the ones of the FDTD solver at very high order. Tests on other wavelengths and time steps (not shown here) show the same trend.

There is generally a good agreement between the analytical calculation (represented by solid lines) and the numerical results (represented by markers), but with some small discrepancies at higher orders. The discrepancies are believed to come from the calculation of the angular wavelength using equation 3.25 which assumes that k_x and k_y are independent of the position in the grid. Evaluation of improved analytical estimates that take those effects into account is left for future work.

5. Conclusion

Theoretical and numerical analysis of the coefficient of reflection of PML layers have been extended to solvers of any order of accuracy, including at the

limit of the infinite order that represents the pseudo-spectral formulations. Results from the analysis, confirmed by numerical simulations, show that the efficiency of PML layers is preserved at high order, and with the PSTD solver.

The analytical expressions that were developed in this paper can be used to predict the coefficients of reflection in various situations with relatively high accuracies. This provides a tool for optimizing the absorption profile in PML layers. Methods for more accurate predictions are under development.

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Appendix A. Derivation of the coefficient of reflection at the grid nodes

The explicit derivation of the coefficient of reflection at the grid nodes is given in this appendix for the second order case, where we consider

$$C_N = \begin{cases} 1, & \text{if } N = 1, \\ 0, & \text{otherwise,} \end{cases} \quad (\text{A.1})$$

The set of equations (3.12-3.14) is solved by first differencing 3.13 in time, giving

$$\begin{aligned} E y_{i+1,j+1/2}^n & - E y_{i+1,j+1/2}^{n-1} \\ & = E y_{i,j+1/2}^n - E y_{i,j+1/2}^{n-1} \\ & \quad + \frac{\Delta x}{\Delta y} \left(E x_{i+1/2,j+1}^n - E x_{i+1/2,j}^n - E x_{i+1/2,j+1}^{n-1} + E x_{i+1/2,j}^{n-1} \right) \\ & \quad - \frac{\Delta x}{\Delta t} \left(B z_{i+1/2,j+1/2}^{n+1/2} - 2 B z_{i+1/2,j+1/2}^{n-1/2} + B z_{i+1/2,j+1/2}^{n-3/2} \right), \end{aligned} \quad (\text{A.2})$$

followed by differencing 3.14 according to the transverse y -direction,

$$\begin{aligned} E x_{i+1/2,j+1}^n & - E x_{i+1/2,j}^n \\ & = E x_{i+1/2,j+1}^{n-1} - E x_{i+1/2,j}^{n-1} \\ & \quad + V_y \left(B z_{i+1/2,j+3/2}^{n-1/2} - 2 B z_{i+1/2,j+1/2}^{n-1/2} + B z_{i+1/2,j-1/2}^{n-1/2} \right). \end{aligned} \quad (\text{A.3})$$

Eliminating E_x in Equation A.2 by using A.3, yields

$$\begin{aligned}
E y_{i+1,j+1/2}^n & - E y_{i+1,j+1/2}^{n-1} \\
& = E y_{i,j+1/2}^n - E y_{i,j+1/2}^{n-1} \\
& \quad + \frac{\Delta x}{\Delta y} V_y \left(B z_{i+1/2,j+3/2}^{n-1/2} - 2 B z_{i+1/2,j+1/2}^{n-1/2} + B z_{i+1/2,j-1/2}^{n-1/2} \right) \\
& \quad - \frac{\Delta x}{\Delta t} \left(B z_{i+1/2,j+1/2}^{n+1/2} - 2 B z_{i+1/2,j+1/2}^{n-1/2} + B z_{i+1/2,j+1/2}^{n-3/2} \right).
\end{aligned} \tag{A.4}$$

Differencing then A.4 in the longitudinal x -direction, gives

$$\begin{aligned}
E y_{i+1,j+1/2}^n & - E y_{i+1,j+1/2}^{n-1} - E y_{i,j+1/2}^n + E y_{i,j+1/2}^{n-1} \\
& = E y_{i,j+1/2}^n - E y_{i,j+1/2}^{n-1} - E y_{i-1,j+1/2}^n + E y_{i-1,j+1/2}^{n-1} \\
& \quad + \frac{\Delta x}{\Delta y} V_y \left(B z_{i+1/2,j+3/2}^{n-1/2} - 2 B z_{i+1/2,j+1/2}^{n-1/2} + B z_{i+1/2,j-1/2}^{n-1/2} \right) \\
& \quad - \frac{\Delta x}{\Delta y} V_y \left(B z_{i-1/2,j+3/2}^{n-1/2} - 2 B z_{i-1/2,j+1/2}^{n-1/2} + B z_{i-1/2,j-1/2}^{n-1/2} \right) \\
& \quad - \frac{\Delta x}{\Delta t} \left(B z_{i+1/2,j+1/2}^{n+1/2} - 2 B z_{i+1/2,j+1/2}^{n-1/2} + B z_{i+1/2,j+1/2}^{n-3/2} \right) \\
& \quad + \frac{\Delta x}{\Delta t} \left(B z_{i-1/2,j+1/2}^{n+1/2} - 2 B z_{i-1/2,j+1/2}^{n-1/2} + B z_{i-1/2,j+1/2}^{n-3/2} \right).
\end{aligned} \tag{A.5}$$

Finally, Equation 3.12 is used to eliminate B_z from A.5, giving

$$\begin{aligned}
E y_{i,j+1/2}^{n+1} - E y_{i,j+1/2}^n & = E y_{i,j+1/2}^n - E y_{i,j+1/2}^{n-1} \\
& \quad + \alpha_y \left(E y_{i,j+1/2}^n - 2 E y_{i,j+1/2}^{n-1} + E y_{i,j+1/2}^{n-2} \right) \\
& \quad - \alpha_y \frac{\Delta t}{\Delta y} V_y \left(E y_{i,j+3/2}^{n-1} - 2 E y_{i,j+1/2}^{n-1} + E y_{i,j-1/2}^{n-1} \right) \\
& \quad + \frac{\Delta t}{\Delta y} V_y \left(E y_{i,j+3/2}^n - 2 E y_{i,j+1/2}^n + E y_{i,j-1/2}^n \right) \\
& \quad + \beta_y \frac{\Delta t}{\Delta x} \left(E y_{i+1,j+1/2}^n - 2 E y_{i,j+1/2}^n + E y_{i-1,j+1/2}^n \right) \\
& \quad - \beta_y \frac{\Delta t}{\Delta x} \left(E y_{i+1,j+1/2}^{n-1} - 2 E y_{i,j+1/2}^{n-1} + E y_{i-1,j+1/2}^{n-1} \right).
\end{aligned} \tag{A.6}$$

Expression A.6 now contains only one component E_y , enabling the substitution of a plane monochromatic traveling wave trial-solution for the evaluation of the coefficient of reflection, r_{node} . Assuming a trial solution of the form $e^{i\omega\Delta t - i(k_x\Delta x + k_y\Delta y)}$, and that the norms of k_x and k_y are conserved by the transmitted and the reflected waves, the transmitted wave is given by $(1 - r)e^{i\omega\Delta t - i(k_x\Delta x + k_y\Delta y)}$, and the signal in front of the slice in x -direction is defined

as a sum of the incident wave and the reflected one, giving $e^{i\omega\Delta t - i(k_x\Delta x + k_y\Delta y)} - re^{i\omega\Delta t + i(k_x\Delta x + k_y\Delta y)}$ (where r represents the coefficient of reflection). Considering a slice at i , we have

$$\begin{aligned}
Ey_{i,j+1/2}^{n+1} &= (1-r)e^{i\omega\Delta t - i(k_y\Delta y/2)}, \\
Ey_{i,j+1/2}^n &= (1-r)e^{-i(k_y\Delta y/2)}, \\
Ey_{i,j+1/2}^{n-1} &= (1-r)e^{-i\omega\Delta t - i(k_y\Delta y/2)}, \\
Ey_{i,j+1/2}^n &= (1-r)e^{-i(k_y\Delta y/2)}, \\
Ey_{i,j+1/2}^{n-1} &= (1-r)e^{-i\omega\Delta t - i(k_y\Delta y/2)}, \\
Ey_{i,j+1/2}^{n-2} &= (1-r)e^{-2i\omega\Delta t - i(k_y\Delta y/2)}, \\
Ey_{i,j+3/2}^{n-1} &= (1-r)e^{-i\omega\Delta t - i(3k_y\Delta y/2)}, \\
Ey_{i,j-1/2}^{n-1} &= (1-r)e^{-i\omega\Delta t - i(-k_y\Delta y/2)}, \\
Ey_{i,j+3/2}^n &= (1-r)e^{-i(3k_y\Delta y)/2}, \\
Ey_{i+1,j+1/2}^n &= (1-r)e^{-i(-k_x\Delta x - k_y\Delta y)/2}, \\
Ey_{i+1,j+1/2}^{n-1} &= (1-r)e^{-i\omega\Delta t - i(-k_x\Delta x - k_y\Delta y)/2}, \\
Ey_{i-1,j+1/2}^n &= e^{-i(-k_x\Delta x + k_y\Delta y/2)} - re^{-i(k_x\Delta x + k_y\Delta y/2)}, \\
Ey_{i-1,j+1/2}^{n-1} &= e^{-i\omega\Delta t - i(-k_x\Delta x + k_y\Delta y/2)} - re^{-i\omega\Delta t - i(k_x\Delta x + k_y\Delta y/2)}. \quad (\text{A.7})
\end{aligned}$$

Inserting the plane monochromatic traveling-wave trial solutions of A.7 in equation A.6, and solving yields the coefficient of reflection at the grid nodes, r_{node} .

$$r_{node} = \frac{a - b \cos(k_y\Delta y) - c \cos(k_x\Delta x)}{a - \cos(k_y\Delta y) - ce^{-ik_x\Delta x}}, \quad (\text{A.8})$$

where

$$\begin{cases} a &= e^{i\omega\Delta t} - (2 + \alpha_y) + e^{-i\omega\Delta t} (1 + 2\alpha_y) + \alpha_y e^{-2i\omega\Delta t}, \\ b &= 2V_y \frac{\Delta t}{\Delta y} (1 - \alpha_y e^{-i\omega\Delta t}), \\ c &= 2\beta_y \frac{\Delta t}{\Delta x} (1 - e^{-i\omega\Delta t}). \end{cases}$$

Appendix B. Derivation of the coefficient of the reflection at the grid inter-nodes

The explicit derivation of the coefficient of reflection at the grid nodes is given in this appendix for the second order case, where we consider

$$C_N = \begin{cases} 1, & \text{if } N = 1, \\ 0, & \text{otherwise.} \end{cases} \quad (\text{B.1})$$

The set of equations (3.15-3.19) is solved by first differencing 3.18 in time, giving

$$\begin{aligned} \text{Bzx}_{i+1/2,j+1/2}^{n+1/2} - \text{Bzx}_{i+1/2,j+1/2}^{n-1/2} &= \alpha_x^* \left(\text{Bzx}_{i+1/2,j+1/2}^{n-1/2} - \text{Bzx}_{i+1/2,j+1/2}^{n-3/2} \right) \\ &\quad - \beta_x^* \left(\text{Ey}_{i+1,j+1/2}^n - \text{Ey}_{i,j+1/2}^n - \text{Ey}_{i+1,j+1/2}^{n-1} + \text{Ey}_{i,j+1/2}^{n-1} \right). \end{aligned} \quad (\text{B.2})$$

Then, by using $\text{Bzx}_{i+1/2,j+1/2}^{n+1/2} = \text{Bz}_{i+1/2,j+1/2}^{n+1/2} - \text{Bzy}_{i+1/2,j+1/2}^{n+1/2}$ in B.3, we get

$$\begin{aligned} \text{Bz}_{i+1/2,j+1/2}^{n+1/2} - \text{Bz}_{i+1/2,j+1/2}^{n-1/2} &= \alpha_x^* \left(\text{Bz}_{i+1/2,j+1/2}^{n-1/2} - \text{Bz}_{i+1/2,j+1/2}^{n-3/2} \right) \\ &\quad - \alpha_x^* \left(\text{Bzy}_{i+1/2,j+1/2}^{n+1/2} - \text{Bzy}_{i+1/2,j+1/2}^{n-1/2} \right) \\ &\quad + \text{Bzy}_{i+1/2,j+1/2}^{n-1/2} - \text{Bzy}_{i+1/2,j+1/2}^{n-3/2} \\ &\quad - \beta_x^* \left(\text{Ey}_{i+1,j+1/2}^n - \text{Ey}_{i,j+1/2}^n - \text{Ey}_{i+1,j+1/2}^{n-1} + \text{Ey}_{i,j+1/2}^{n-1} \right). \end{aligned} \quad (\text{B.3})$$

Using equation 3.19, we obtain

$$\begin{aligned} \text{Bz}_{i+1/2,j+1/2}^{n+1/2} - \text{Bz}_{i+1/2,j+1/2}^{n-1/2} &= \alpha_x^* \left(\text{Bz}_{i+1/2,j+1/2}^{n-1/2} - \text{Bz}_{i+1/2,j+1/2}^{n-3/2} \right) \\ &\quad - \alpha_x^* \frac{\Delta t}{\Delta y} \left(\text{Ex}_{i+1/2,j+1}^{n-1} - \text{Ex}_{i+1/2,j}^{n-1} \right) \\ &\quad + \frac{\Delta t}{\Delta y} \left(\text{Ex}_{i+1/2,j+1}^n - \text{Ex}_{i+1/2,j}^n \right) \\ &\quad - \beta_x^* \left(\text{Ey}_{i+1,j+1/2}^n - \text{Ey}_{i,j+1/2}^n - \text{Ey}_{i+1,j+1/2}^{n-1} + \text{Ey}_{i,j+1/2}^{n-1} \right). \end{aligned} \quad (\text{B.4})$$

In order to express equation B.4 only by B_z components, we eliminate E_y and E_x by differencing in time and by substituting E_y of equation 3.16 and E_x of equation 3.15, which gives

$$\begin{aligned}
Bz_{i+1/2,j+1/2}^{n+1/2} & - Bz_{i+1/2,j+1/2}^{n-1/2} \\
& = Bz_{i+1/2,j+1/2}^{n-1/2} - Bz_{i+1/2,j+1/2}^{n-3/2} \\
& \quad + \alpha_x^* \left(Bz_{i+1/2,j+1/2}^{n-1/2} - 2Bz_{i+1/2,j+1/2}^{n-3/2} + Bz_{i+1/2,j+1/2}^{n-5/2} \right) \\
& \quad - \alpha_x^* V_y \frac{\Delta t}{\Delta y} \left(Bz_{i+1/2,j+3/2}^{n-3/2} - 2Bz_{i+1/2,j+1/2}^{n-3/2} + Bz_{i+1/2,j-1/2}^{n-3/2} \right) \\
& \quad + V_y \frac{\Delta t}{\Delta y} \left(Bz_{i+1/2,j+3/2}^{n-1/2} - 2Bz_{i+1/2,j+1/2}^{n-1/2} + Bz_{i+1/2,j-1/2}^{n-1/2} \right) \\
& \quad + \beta_x^* V_x \left(Bz_{i+3/2,j+1/2}^{n-1/2} - 2Bz_{i+1/2,j+1/2}^{n-1/2} + Bz_{i-1/2,j+1/2}^{n-1/2} \right) \\
& \quad - \beta_x^* V_x \left(Bz_{i+3/2,j+1/2}^{n-3/2} - 2Bz_{i+1/2,j+1/2}^{n-3/2} + Bz_{i-1/2,j+1/2}^{n-3/2} \right). \tag{B.5}
\end{aligned}$$

Assuming a plane monochromatic traveling-wave trial solution of the form $e^{i\omega\Delta t - i(k_x\Delta x + k_y\Delta y)}$, one has

$$\begin{aligned}
Bz_{i+1/2,j+1/2}^{n+1/2} & = (1-r)e^{i\omega\Delta t/2 - i(k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i+1/2,j+1/2}^{n-1/2} & = (1-r)e^{-i\omega\Delta t/2 - i(k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i+1/2,j+1/2}^{n-3/2} & = (1-r)e^{-3i\omega\Delta t/2 - i(k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i+1/2,j+1/2}^{n-5/2} & = (1-r)e^{-5i\omega\Delta t/2 - i(k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i+1/2,j+3/2}^{n-3/2} & = (1-r)e^{-3i\omega\Delta t/2 - i(k_x\Delta x + 3k_y\Delta y)/2}, \\
Bz_{i+1/2,j-1/2}^{n-3/2} & = (1-r)e^{-3i\omega\Delta t/2 - i(k_x\Delta x - k_y\Delta y)/2}, \\
Bz_{i+1/2,j+3/2}^{n-1/2} & = (1-r)e^{-i\omega\Delta t/2 - i(k_x\Delta x + 3k_y\Delta y)/2}, \\
Bz_{i+1/2,j-1/2}^{n-1/2} & = (1-r)e^{-i\omega\Delta t/2 - i(k_x\Delta x - k_y\Delta y)/2}, \\
Bz_{i+3/2,j+1/2}^{n-1/2} & = (1-r)e^{-i\omega\Delta t/2 - i(3k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i+3/2,j+1/2}^{n-3/2} & = (1-r)e^{-3i\omega\Delta t/2 - i(3k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i-1/2,j+1/2}^{n-1/2} & = e^{-i\omega\Delta t/2 - i(-k_x\Delta x + k_y\Delta y)/2} - re^{-i\omega\Delta t/2 - i(k_x\Delta x + k_y\Delta y)/2}, \\
Bz_{i-1/2,j+1/2}^{n-3/2} & = e^{-3i\omega\Delta t/2 - i(-k_x\Delta x + k_y\Delta y)/2} - re^{-3i\omega\Delta t/2 - i(k_x\Delta x + k_y\Delta y)/2}, \tag{B.6}
\end{aligned}$$

By inserting the plane monochromatic traveling-wave trial solutions of B.6 in equation B.5, we deduce the coefficient of reflection on the inter-node,

$r_{inter-node}$.

$$r_{inter-node} = \frac{a - b \cos(k_y \Delta y) - c \cos(k_x \Delta x)}{a - \cos(k_y \Delta y) - c e^{-i k_x \Delta x}}, \quad (\text{B.7})$$

where

$$\begin{cases} a &= e^{i\omega \Delta t} - (2 + \alpha_y^*) + e^{-i\omega \Delta t} (1 + 2\alpha_y^*) + \alpha_y^* e^{-2i\omega \Delta t}, \\ b &= 2V_y \frac{\Delta t}{\Delta y} (1 - \alpha_y^* e^{-i\omega \Delta t}), \\ c &= 2\beta_y^* \frac{\Delta t}{\Delta x} (1 - e^{-i\omega \Delta t}). \end{cases}$$

Appendix C. Summary

The coefficient of reflection on the full-node at each plane of the layer, r_{node} are summarized in the following table:

Order of accuracy	Plane wave at normal incidence (1D)	Plane wave at oblique incidence (2D)
2	$r_{node} = \frac{a-b(-1+\cos(k\Delta x))}{a-b(-1+e^{-ik\Delta x})}$	$r_{node} = \frac{a-b \cos(k_y \Delta y) - c \cos(k_x \Delta x)}{a - \cos(k_y \Delta y) - c e^{-i k_x \Delta x}}$
> 2	$r_{node} = \frac{a-b \sum_{N=0}^{\infty} \text{Ccoupled}_N \cos N k \Delta x}{a-b \sum_{N=0}^{\infty} \text{Ccoupled}_N e^{-i N k \Delta x}}$	$r_{node} = \frac{a-b \sum_{N=0}^{\infty} \text{Ccoupled}_N \cos N k_y \Delta y - c \sum_{N=0}^{\infty} \text{Ccoupled}_N \cos N k_x \Delta x}{a-b \sum_{N=0}^{\infty} \text{Ccoupled}_N \cos N k_y \Delta y - c \sum_{N=0}^{\infty} \text{Ccoupled}_N e^{-i N k_x \Delta x}}$

Table C.2: Summary

where in 1D,

$$\begin{cases} a &= e^{i\omega \Delta t} - 1 - \alpha + \alpha e^{-i\omega \Delta t}, \\ b &= 2\beta V, \end{cases}$$

and in 2D,

$$\begin{cases} a &= e^{i\omega \Delta t} - (2 + \alpha_y) + e^{-i\omega \Delta t} (1 + 2\alpha_y) + \alpha_y e^{-2i\omega \Delta t}, \\ b &= 2V_y \frac{\Delta t}{\Delta y} (1 - \alpha_y e^{-i\omega \Delta t}), \\ c &= 2\beta_y \frac{\Delta t}{\Delta x} (1 - e^{-i\omega \Delta t}). \end{cases}$$