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Space-time PML and Subgrid Connections for Finite Integration Method

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The perfectly matched layer (PML) absorbing boundary is employed in the space-time finite integration (FI) method. Subgrid connections in 3D and 4D space-time are considered. Using the PML, the computational accuracy for 3D and 4D space-time subgrid methods are evaluated. The subgrid scheme given by the space-time FI method suppresses unphysical wave reflections compared with the subgrid scheme based on the spatial FI method.

Index Terms—Boundary condition, electromagnetic wave absorption, finite integration method, time-domain analysis.

I. INTRODUCTION

The electromagnetic field analysis of fine structure at sub-wavelength scales is required for advanced electronic and optical devices [1]. The analysis of these devices using the conventional FDTD method [2] incurs large computational cost because the spatial grid should be refined uniformly unless a sophisticated subgrid method [2] is used for an adaptive grid construction.

The finite integration (FI) method [3]–[5] is an alternative choice for time-domain analysis using a spatial adaptive grid that produces a stable subgrid scheme [6]. The space-time FI method [7], [8] is an advanced version of the FI method that enables efficient electromagnetic field computations using an adaptive time-step. Ref. [9] proposed 3D and 4D space-time subgrid methods for the adaptive grid construction and provided comparisons with the spatial FI subgrid scheme [6]. However, the computational accuracy of the space-time subgrid scheme has not as yet been fully examined because only periodic spatial boundary conditions were implemented.

This paper develops the connection scheme to the perfectly matched layer (PML) absorbing boundary condition in the space-time finite integration method using incidence matrices is presented in [8].

II. SPACE-TIME FINITE INTEGRATION METHOD

Points in the coordinate system are denoted by \((w, x, y, z) = (x^0, x^1, x^2, x^3)\) where \(w = ct, c = 1/\sqrt{\varepsilon_0\mu_0}\), and \(\varepsilon_0\) and \(\mu_0\) are the permittivity and permeability of vacuum, respectively. The electromagnetic variables in the FI method are defined as

\[
\partial_\omega \mathbf{F} = 0, \quad \partial_\omega \mathbf{G} = \int_{\Omega_f} \mathbf{J},
\]

where \(\Omega_f\) is the impedance. A

\[
F = -\sum_{i=1}^3 E_i dx^0 dx^i + \sum_{j=1}^3 c B_j dx^k dx^l,
\]

\[
G = \sum_{i=1}^3 H_i dx^0 dx^i + \sum_{j=1}^3 c \mathbf{D}_j dx^k dx^l,
\]

\[
J = c \rho dx^0 dx^2 dx^3 - \sum_{j=1}^3 c J_j dx^0 dx^k dx^l,
\]

where \((j, k, l)\) is a cyclic permutation of \((1, 2, 3)\), and \(\Omega_p\) and \(\Omega_d\) are hypersurfaces in space-time; \(\partial\Omega_p\) and \(\partial\Omega_d\) denote the faces of the primal and dual grids, respectively; \(\rho\) is the electric charge density and \(J_j\) is the electric current density. The electromagnetic variables in the FI method are defined as

\[
f = \int_{\Omega_p} F, g = \int_{\Omega_d} G,
\]

where \(S_p\) and \(S_d\) are the faces of the primal and dual grids \(\partial\Omega_p\) and \(\partial\Omega_d\). To express the constitutive equation simply, the Hodge dual grid [7] is introduced as

\[
\int_{\Omega_d} c_i dx^0 dx^i = \frac{1}{\sqrt{\varepsilon_0\mu_0}} \int_{\Omega_p} c_i dx^0 dx^i = \kappa,
\]

where \(\kappa = 1/\sqrt{\varepsilon_0\mu_0}\). A

III. PML ABSORBING BOUNDARY CONDITION

In the 3D space, all the components of the electric flux density and the magnetic flux density are divided into two subcomponents respectively such that

\[
D_x = D_{xy} + D_{xz},
\]

where \(D_{xy}\) and \(D_{xz}\) are the respective components of \(D_x\) propagating along the \(y\) and \(z\)-directions. Using these subcomponents, the space-time FI method updates the electric flux density in the PML as

\[
d_{xy,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} = \frac{1}{1 + \frac{\Delta w}{2} \sigma x Z} \left( h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} - h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} \right) + \frac{1}{1 + \frac{\Delta w}{2} \sigma z Z} \left( h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} - h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} \right),
\]

\[
d_{xz,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} = \frac{1}{1 + \frac{\Delta w}{2} \sigma z Z} \left( h_{z,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} - h_{z,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} \right),
\]

\[
d_{xx,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} = \frac{1}{1 + \frac{\Delta w}{2} \sigma z Z} \left( h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} - h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} \right) - \frac{1}{1 + \frac{\Delta w}{2} \sigma z Z} \left( h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} - h_{x,i-\frac{1}{2}j-\frac{1}{2}k-\frac{1}{2}} \right),
\]

where

\[
\frac{\Delta w}{2} \sigma Z
\]
where $\sigma_x$ and $\sigma_z$ are the electric conductivities in the $y$ and $z$-directions, respectively, $\Delta w$ is the time-step, the subscripts are spatial indices for the $x$, $y$, and $z$ directions, and the superscript is the temporal index. The time-marching scheme for the other variables is given similarly.

This section gives an explicit description of the connecting variables.

Fig. 1. 3D space-time subgrid of straight type: (a) corner part and (b) space-time connection.

Fig. 2. 3D space-time subgrid of staircase type: (a) spatial and (b) space-time connections.

Fig. 3. Computational domain showing subgrid and PML.

Fig. 4. Discrepancy of $B_3$ compared with FDTD method: (a) $\delta=0.01$ and (b) $\delta=0.1$.

IV. SPACE-TIME SUBGRID CONNECTION

Ref. [9] proposed straight-type and staircase-type subgrids in the 3D and 4D space-times. However, the subgrid connection in 4D space-time was not discussed in detail because the 4D geometry is not always intuitively explainable. This section gives an explicit description of the connecting faces at the subgrid boundary.

A. 3D space-time subgrid

The 3D straight-type and staircase-type space-time subgrids are examined with the PML boundary condition. Fig. 1 illustrates the straight-type subgrid connection, where $\delta$ is a free parameter to locate the subgrid boundary. Ref. [9] proposed the staircase-type subgrid connection (Fig. 2) bending the edges and faces of the space-time grid.

Fig. 3 illustrates the computational domain having the subgrid and PML. For simplicity, the permittivity and permeability are set uniformly to unity by the normalization replacing the variable $F$ by $F/\sqrt{\mu_0/\varepsilon_0}$. The coordinates are linearly transformed to normalize $\Delta x$ to 1; the normalized temporal step $\Delta w$ is set to 0.5. The normalized initial conditions are $E_1 = E_2 = 0$ and $B_3 = \exp\left\{-(x^1)^2+(x^3)^2\right\}/25$. Fig. 4 depicts the distributions of discrepancy $\Delta B_3$ between $B_3$ obtained employing the FDTD method and that obtained using the 3D staircase-type space-time subgrid at $ct=100$ with $\delta=0.01$ and 0.1. Unphysical wave reflection caused by the subgrid connection is reduced by the optimization of $\delta$.

B. 4D Straight-type subgrid

We use bases $dx_i$ satisfying $dx_i dx_j = \delta_{ij}$ to represent edges and $dx_i/dx_j$ to represent faces having subscripts $i, j = 0, 1, 2, 3$, where $\wedge$ denotes the wedge product.

Fig. 5 illustrates the straight-type subgrid connection, where eight edges connect the node $P: (0, 0, 0, 0)$ on the coarse grid side and the eight nodes $Q_{0, \pm 1, \pm 1, \pm 1}$ on the fine grid side of dual grid. The edge to node $Q_{1, 1, 1, 1}$ from $P$ is represented as $\Delta x(3dx_1/4 - dx_2/4 - dx_3/4) - \Delta w dx_0/4$. This edge belongs to the faces $S_{0i}$ ($i = 1, \ldots, 4$) of the dual grid, which are represented as

$$
S_{d1} = \frac{3\Delta w}{4} dx_0 \wedge \left[ \Delta x \left( \frac{3}{4} dx_1 - \frac{1}{4} dx_2 - \frac{1}{4} dx_3 - \frac{\Delta w}{4} dx_0 \right) \right],$$

$$
S_{d2} = \frac{\Delta w}{4} dx_0 \wedge \left[ \Delta x \left( \frac{3}{4} dx_1 - \frac{1}{4} dx_2 - \frac{1}{4} dx_3 - \frac{\Delta w}{4} dx_0 \right) \right].
$$

(9)
Based on (6), the corresponding faces $S_{pi}$ $(i = 1, ..., 4)$ of the primal grid are slanted:

$$S_{p1} = \frac{\Delta x}{4}(\frac{1}{4}dx_1 - \frac{1}{4}dx_2 - \frac{1}{4}dx_3 - \frac{\Delta w}{4}dx_0) \wedge \frac{\Delta x}{4}dx_3,$$

$$S_{p2} = \frac{\Delta x}{4}(\frac{1}{4}dx_1 - \frac{1}{4}dx_2 - \frac{1}{4}dx_3 - \frac{\Delta w}{4}dx_0) \wedge \frac{\Delta x}{4}dx_2,$$

$$S_{p3} = \frac{\Delta w}{2}dx_0 - \frac{(c_\delta \Delta w)^2}{6dx_0} dx_1 \wedge \frac{\Delta x}{2}dx_2 + \frac{1}{6}dx_3),$$

$$S_{p4} = \frac{\Delta x}{2}dx_0 - \frac{(c_\delta \Delta w)^2}{6dx_0} dx_1 \wedge \frac{\Delta x}{2}dx_3 + \frac{1}{6}dx_2).$$

Of the variables $f_1 = \int_{S_1} F$ and $g_1 = \int_{S_2} G$ $(i = 1, ..., 4)$, $f_1$ and $f_2$ denote the magnetic fluxes whereas $g_1$ and $g_2$ are the magnetomotive forces with

$$f_1 = (\Delta x)^2 \frac{3}{6c_1 - b_2 - c_3},$$

$$g_1 = 3\Delta x^w \frac{1}{6} H_1 - H_2 - H_3 = \frac{9c_1 \Delta w f_1}{4\Delta x},$$

The dominant component of $f_1$ and $f_2$ is the electromotive force but also contain magnetic fluxes such that

$$f_3 = \Delta w \frac{-\Delta x(3c_2 + E_z) - \Delta w c_1 c_2}{12},$$

Similarly, the dominant component of $g_1$ and $g_2$ is the electric flux but $g_1$ and $g_2$ also include a magnetomotive force dependence such that

$$g_3 = 3\Delta w \frac{-\Delta x(3c_2 + 3c_1 - \Delta w H_3)}{4c_2 \Delta w}.  \tag{16}$$

C. 4D Staircase type subgrid

Fig. 6 illustrates the staircase-type subgrid connection, where the edges from node $P$ to nodes $Q_{i\pm\pm}$ are bent at the points $R_{\pm\pm\pm}$: $(\pm \Delta x/4, 0, \pm \Delta y/4, \pm \Delta z/4)$. Consequently, the face $S_{d11}$ has different direction from $S_{d2}$ as

$$S_{d1} = \Delta x \Delta w \left(\frac{3}{16} dx_0 dx_1 - \frac{3}{16} dx_0 dx_2 + \frac{3}{16} dx_0 dx_3 \right),$$

$$S_{d2} = \Delta x \Delta w \left(\frac{3}{16} dx_0 dx_1 - \frac{3}{16} dx_0 dx_2 + \frac{3}{16} dx_0 dx_3 \right).  \tag{17}$$

The face $S_{d2}$ also has a different direction from $S_{d3}$,

$$S_{d3} = (\Delta x)^2 \left(-\frac{3}{8} dx_3 dx_1 - \frac{3}{16} dx_3 dx_2 \right),$$

$$S_{d4} = (\Delta x)^2 \left(-\frac{3}{8} dx_3 dx_1 - \frac{3}{16} dx_3 dx_2 \right).$$

Based on (6), the corresponding faces $S_{pi}$ $(i = 1, ..., 4)$ are slanted:

$$S_{p1} = (\Delta x)^2 \left(\frac{1}{4} dx_2 dx_3 + \frac{1}{8} dx_2 dx_1 - \frac{1}{8} dx_1 dx_2 \right),$$

$$S_{p2} = (\Delta x)^2 \left(\frac{1}{4} dx_2 dx_3 - \frac{1}{2} dx_1 dx_0 - \frac{1}{2} dx_1 dx_2 \right),$$

$$S_{p3} = \Delta x \Delta w \left(\frac{1}{4} dx_0 dx_2 + \frac{1}{8} dx_1 dx_0 \right) - (c_\delta \Delta w)^2 \frac{1}{8} dx_1 dx_2,$$

$$S_{p4} = \Delta x \Delta w \left(\frac{1}{4} dx_0 dx_2 + \frac{1}{16} dx_0 dx_1 \right) - (c_\delta \Delta w)^2 \frac{1}{24} dx_1 dx_2.  \tag{20}$$

D. Corner correction

Ref. [11] proposed a symmetric correction for the corner variables (Fig. 7), where the orthogonality (6) may not be satisfied. The electromotive forces ($e_x$, $e_y$, and the electric fluxes ($d_x$, $d_y$) are given by the first and second of (5), respectively. When the parameter $\delta \neq 0$, the face for $e_x$ (or $e_y$) is not orthogonal to the face for $d_x$ ($d_y$). Based on the vectorial relation [Fig. 7(b)], a symmetric correction is appropriate:

$$\begin{align*}
\begin{pmatrix} e_x \\ e_y \end{pmatrix} &= \frac{\Delta w}{\Delta x} \begin{pmatrix} 1 & -\delta' \\ -\delta' & 1 - \delta \end{pmatrix}^{-1} \begin{pmatrix} d_x \\ d_y \end{pmatrix},
\end{align*} \tag{21}$$

having no asymmetry arising in the impedance matrix. Because the face for $e_x$ ($e_y$) is slanted along the $x$-direction (Fig. 5), $\delta'$ is given by $\delta + (c_\delta \Delta w)^2/(12 \Delta x)$ for the straight-type grid. The magnetic variables at the corners are similarly corrected symmetrically,

$$\begin{align*}
\begin{pmatrix} h_x \\ h_y \end{pmatrix} &= \frac{\Delta w}{\Delta x} \begin{pmatrix} 1 & -\delta'' \\ -\delta'' & 1 - \delta'' \end{pmatrix}^{-1} \begin{pmatrix} b_x \\ b_y \end{pmatrix},
\end{align*} \tag{22}$$

where ($b_x$, $b_y$) and ($h_x$, $h_y$) are the magnetic fluxes and magnetomotive forces and $\delta'' = \delta - \Delta x/12$. An eigenvalue analysis [11] showed that the 4D subgrid schemes for the straight and staircase types are conditionally stable with and without the symmetric correction.
V. NUMERICAL ASSESSMENT

The waveguide (Fig. 8) is used to evaluate the 4D staircase-type subgrid scheme with corner corrections with δ = 0.12. For simplicity, the permittivity and permeability are set uniformly to unity by normalization in the same way as in IV.A. The normalized spatial domain size is 240 × 48 × 24 including a subgrid domain of 120 \( \leq x^1 \leq 180\), 12 \( \leq x^2 \leq 36\), and 6 \( \leq x^3 \leq 18\). The inlet field values are given to excite the TE_{10} mode. The PML absorbing boundary condition is applied at the exit.

Figs. 9(a) and (b) shows the propagation of the incident wave \( E_x^{in} \) and \( B_z^{in} \), respectively, at \( x^0 = 240\), which is simulated with (\( \Delta x, \Delta \omega \)) = (1, 0.4); the normalized frequency is 0.05 measured by the normalized coordinate \( x^i \). Fig. 9(c) depicts the propagation of the reflected wave \( B_z^r \) at \( x^i = 240\), which is unphysically yielded by the subgrid connection at \( x^i = 120\). For comparison, Fig. 9(d) shows the reflected wave obtained by the subgrid scheme based on the spatial FI method given in [6]. The space-time FI subgrid reduces the maximal \( |B_z^r| \) by a factor of 0.4 compared with the spatial FI scheme.

To evaluate theses unphysical reflections, the Poynting vectors of the incidence and reflected waves are averaged along the \( x^1-x^2 \) cross-section; these vectors are denoted by \( P^r(x^i) \) and \( P^i(x^i) \), respectively and their maximal absolute values along the \( x^1 \)-direction are \( P_{max}^r \) and \( P_{max}^i \). Fig. 10 compares the square root of \( P_{max}^r/P_{max}^i \). Obtained by the spatial FI subgrid scheme and the proposed space-time FI subgrid, where (\( \Delta x, \Delta \omega \)) = (2, 0.8), (1, 0.4), (0.5, 0.2) and three subgrid domains below are examined:

(a) \([120, 180] \times [12, 36] \times [6, 18]\),
(b) \([140, 200] \times [16, 40] \times [6, 18]\),
(c) \([140, 200] \times [12, 36] \times [8, 20]\).

For comparison, Fig. 10 also shows the result given by the space-time FI subgrid without the corner correction and with \( \delta = 0.08\). The space-time FI subgrid scheme yields smaller unphysical wave reflections than the spatial FI subgrid. The corner correction improves the accuracy.

VI. CONCLUSION

The PML absorbing boundary condition is introduced in a natural manner into the space-time FI method. The 4D space-time subgrid connections of the straight and staircase types are discussed in the framework of the Hodge dual grid. The space-time FI method using the staircase-type subgrid reduces unphysical wave reflection compared with the conventional subgrid based on the spatial FI method.

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