Dispersion optimised plane wave sources for scattering analysis with integral based high order finite difference time domain methods

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Abstract: The implementation of plane wave incidence using the total-field/scattered-field (TFSF) formulation for a three-dimensional finite volumes-based, extended-stencil finite-difference time-domain (FV24) algorithm is presented. This achievement required designing an auxiliary one-dimensional grid with the characteristics of (i) co-located electric field components uniformly spaced from co-located magnetic field components, (ii) grid spacing that dynamically changes with desired angles of propagation to eliminate the need for field interpolations when mapping the plane wave to the main grid, (iii) update equations that precisely match the numerical dispersion characteristics of the main FV24 algorithm, and (iv) auxiliary to main grid field mapping that encompasses six parallel surfaces along the TFSF boundary to satisfy the extended cell nature of the main FV24 algorithm. The resulting non-physical field leakage into the scattered-field region is observed to be independent of angle of incidence and has a ~300 dB noise floor. This technique extends the high-order FV24 capabilities to include accurate and efficient simulations of electrically large scatterers using relatively low grid densities, bringing this capability to today’s desk-side workstations.

1 Introduction

The finite-volumes based finite-difference time-domain (FDTD) (FV24) algorithm [1] is a high-order FDTD method designed to counter the effect of relatively large phase errors in propagated waves when a coarse grid is used. This drawback is further exacerbated in traditional FDTD by the wild swings in phase error levels as scattered waves propagate in multiple directions. When FDTD is used to model electrically large problems, super-fine grids are required that need to get ever denser the larger the problem gets. The end result is a quickly approached computing resources ceiling that limits FDTD’s applicability to moderate-sized problem at best. High-order FDTD variants aim, in general, to provide controlled and greatly reduced phase errors when using grid resolutions in the order of 10–20 cells per wavelength for modelling problem sizes ranging from dozens to hundreds of wavelengths. Comparisons with other high-order algorithms have demonstrated that the FV24 and its two-dimensional (2D) version, the M24 algorithm [2], exhibit the highest level of phase preservation performance [1, 3]. Another advantage to the FV24 algorithm over other high-order FDTD algorithms is the continued development it has received in the form of specially designed modelling tools that preserve the algorithm’s phase performance. Examples of these tools are the convolutional perfectly-matched-layer absorbing boundary conditions [4], conformal perfect-electric-conductor modelling [5] and graphical processing units code optimisation [6].

A critical modelling tool that is yet to be developed for the FV24 algorithm is plane wave injection for simulating scattering problems. An effective approach to introduce this tool is to isolate the scattering object with an enclosing virtual surface and introduce conditions on that surface to excite the required plane wave within its confines while allowing only scattered waves from the object under study to pass through it transparently, thus effecting an excellent dynamic range for the observed scattered fields (see Fig. 1). This technique is referred to as the total-field/scattered-field (TFSF) method [7]. The most effective TFSF variant to-date is the one-dimensional (1D) MAP technique [8, 9] which uses a 1D auxiliary array that is designed to propagate a plane wave with an identical numerical behaviour properties to that of the main hosting grid, thus allowing seamless cross-mapping with virtually no leakage of non-scattered fields outside the TFSF virtual surface. Since its introduction, the 1D MAP has been extended to the 2D M24 high-order algorithm [10] and a basic three-dimensional (3D) high-order FDTD variant [11]. This paper is concerned with the implementation of the 1D MAP technique within the FV24 algorithm to extend its applicability to modelling electrically large scattering problems such as multiple target detection while in formation or weather system radar simulations. The presentation will start with a simplified graphical explanation of the 1D MAP when implemented in standard 3D FDTD grids. A slightly restricted form of 1D MAP will be discussed to accommodate an efficient subsequent code development. This choice becomes apparent when it is realised that FV24 extended-stencil cells involve additional 36 field nodes to the four used for standard FDTD (see Fig. 2). This is followed by a detailed algorithm development for FV24, code implementation and finally, numerical validation results.

2 1D auxiliary propagator

The central theme behind implementing an error-free plane wave incidence using TFSF formulation is the perfect dispersion-matched 1D auxiliary propagator. This dispersion matching between the auxiliary 1D grid and the main FDTD grid makes it possible to reduce the spurious field leakage into the scattered-field region to the order 10−15 or ~300 dB using double precision computations. One approach for the perfect dispersion matching is to convert the same update equations as that of the main 3D grid into 1D form for propagating the plane wave. The 3D FDTD update equations, for example...
Every $E$ or $H$ field component in the main grid can be projected onto an imaginary axis defined by the vector $P = p_x a_x + p_y a_y + p_z a_z = \cos \theta \sin \phi \mathbf{a}_x + \sin \theta \sin \phi \mathbf{a}_y + \cos \phi \mathbf{a}_z$, where $\theta$ and $\phi$ are the traditionally defined angles within spherical coordinates. As an example, the main grid $E_x$ location $X = (I + (1/2), J, K)$ is projected as $P \cdot X = p_x (I + (1/2)) h + p_y J h + p_z K h$. In the following presentation, we will enforce a minor restriction that would allow us to assemble a unified auxiliary 1D propagator that hosts all six field components where the three electric field components are co-located and leap-frogging the similarly co-located magnetic field components. This choice furnishes an easy conversion of algorithm equations to code indexing as explained in [10]. It also agrees with the established approach of presenting all six field components in a single 3D staggered-field Yee cell [7, 12]. Removing this odd-integer restriction will not invalidate the 1D MAP technique used here. It will however introduce additional overhead when determining index matching between the auxiliary and main grids while coding it. It will also force us to interpret the auxiliary grid as six separate 1D grids similar to Fig. 2 in [9].

If we choose
\[
p_{ih} = p_{jh} = p_{zh} = \Delta x
\]
for some odd integers $m_x$, $m_y$, and $m_z$ (the rational angle condition [9, 10, 13]), then
\[
P \cdot X/\Delta x = m_x(I + 1/2) + m_y J + m_z K = i.
\]
Similarly, the indices for $H_x$ components at $(I + (1/2), J \pm (1/2), K)$ or $H_y$ components at $(I + (1/2), J, K \pm (1/2))$ in (1) are
\[
m_x(I + 1/2) + m_y(J \pm 1/2) + m_z K = i \pm m_y/2
\]
and
\[
m_x(I + 1/2) + m_y J + m_z(K \pm 1/2) = i \pm m_y/2,
\]
respectively. Consequently, all $H$ nodes will map to the 1D grid at integer multiples of $\Delta x$, while all $E$ nodes will map to integer multiples plus $\Delta x/2$. The choice of $m_x$, $m_y$, and $m_z$ will decide the direction of plane wave propagation,
\[
\phi = \tan^{-1} \frac{m_y}{m_x}, \quad \theta = \cos^{-1} \sqrt{\frac{m_z}{m_x^2 + m_y^2 + m_z^2}}.
\]
The projections of all main grid $E$ and $H$ locations and the associated index mapping explained earlier results in a 1D propagator that is arranged in a leap-frog manner of co-located $E_x$, $E_y$, $E_z$ components, followed by co-located $H_x$, $H_y$, $H_z$ components. The spacing between the electric field nodes and between the magnetic field nodes is identically $\Delta x$. Figs. 3 and 4 offer a 3D and a topographical 2D view of $E$ and $H$ projections and highlights the uniformity of the 1D grid for a typical case of $m_x = 5$, $m_y = 3$ and $m_z = 1$. To illustrate, the circled projections in Fig. 4 represent the following combinations assuming location $(0, 0, 0)$ coincides with the lower left corner of the shown grid:

(i) Corresponds to $P \cdot X = (3/2)\Delta x$, the projection of $E_x(0, (1/2), 0)$ and $E_y(0, (2, 3/2))$ among other $E$ components.
(ii) Corresponds to $P \cdot X = 2\Delta x$, the projection of $H_y(0, (1/2), (1/2))$ and $H_z(0, (1/2), (3/2))$ among other $H$ components.
(iii) Corresponds to $P \cdot X = (5/2)\Delta x$, the projection of $E_y((1/2), 0, 0)$ and $E_z((0, 1/2), 1)$ among other $E$ components.
(iv) Corresponds to $P \cdot X = 3\Delta x$, the projection of $H_z((1/2), 0, (1/2))$, $H_z(0, (1/2), (3/2))$ among other $H$ components.
(v) Corresponds to $P \cdot X = (7/2)\Delta x$, the projection of $E_y((1/2), 0, 1)$, $E_z((1/2), 0, 2)$ and $E_z(0, (1/2), 1)$ among other $E$ components.
A code friendly fully integer representation of \( E \) and \( H \) node indexing along the 1D propagator [10] can be written by assuming that the \( E \) components have the same array indices as the \( H \) components that succeed them along the 1D propagator. With this convention, (1) can be finally written as

\[
E_{i,j}^{n+1} = E_{i,j}^n + \Delta t \left[ \frac{H_{i,j+1/2,K}^{n+1/2} - H_{i,j-1/2,K}^{n+1/2}}{\Delta y} \right] - \frac{\Delta t}{\Delta y} \left[ E_{i,j+1/2,K+1}^n - E_{i,j-1/2,K+1}^n \right] - \frac{\Delta t}{\Delta y} \left[ E_{i,j+1/2,K+1}^n - E_{i,j-1/2,K+1}^n \right].
\]

In a similar manner, the main grid update equation for \( H \) is

\[
H_{i,j}^{n+1/2} = H_{i,j}^{n-1/2} + \Delta t \left[ \frac{E_{i,j+1/2,K}^{n+1} - E_{i,j-1/2,K}^{n+1}}{\Delta y} \right] - \frac{\Delta t}{\Delta y} \left[ E_{i,j+1/2,K+1}^{n+1} - E_{i,j-1/2,K+1}^{n+1} \right] - \frac{\Delta t}{\Delta y} \left[ E_{i,j+1/2,K+1}^{n+1} - E_{i,j-1/2,K+1}^{n+1} \right].
\]

translates into the 1D form

\[
H_{i,j}^{n+1/2} = H_{i,j}^{n-1/2} + \Delta t \left[ \frac{E_{i,j+1/2,K}^{n+1} - E_{i,j-1/2,K}^{n+1}}{\Delta y} \right] - \frac{\Delta t}{\Delta y} \left[ E_{i,j+1/2,K+1}^{n+1} - E_{i,j-1/2,K+1}^{n+1} \right] - \frac{\Delta t}{\Delta y} \left[ E_{i,j+1/2,K+1}^{n+1} - E_{i,j-1/2,K+1}^{n+1} \right].
\]

The coefficients in this equation are given by \( c_b\lambda_0 = K_b\Delta y/\epsilon_0 \), \( c_b\lambda_i = K_b\Delta y/\epsilon_i \), \( c_b\lambda_0 = K_b h_\Delta y/\epsilon_0 \), \( c_b\lambda_i = K_b h_\Delta y/\epsilon_i \), where \( K_b \), \( K_i \) are optimised to reduce the global phase error and \( K_i = 1 - K_b - K_i \). Notwithstanding the additional terms, 3D to 1D index correction or mapping process is the same as that outlined for FDTD. The 1D indices for some of the main grid field locations are listed in Tables 1 and 2.

### 3 TFSF jump conditions

Field nodes in both the main grid and the 1D propagator are concurrently updated at each time step. Within the main grid, the objective of maintaining separately the total field and scattered field regions is accomplished through consistency corrections at and around the interface separating them. The interface itself is assumed to be part of the total-field region. Any field node update equation that uses a mix of surrounding nodes from both regions needs to be modified such that all terms of the update equation represent either total fields or scattered fields according to the location of the field node being updated. Therefore, some of the terms therein need to have the plane wave source component added or subtracted to reflect this balancing act before the next time iteration is initiated. The source correction terms are obtained using the mapping process explained in the previous section. The relative location of the 2D44 extended cell under scrutiny with respect to the cubical TFSF interface will dictate which terms need this treatment.

This extended cell nature also means that at each of the six planes of the TFSF cubical interface, there are six parallel layers of field nodes that warrant update equation corrections. This is in direct contrast to traditional FDTD which limits TFSF corrections to only two parallel layers at each interface plane.

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**Fig. 3** 3D view showing projections of all E and H locations onto the 1D propagator for the case \( m_x = 5, m_y = 3 \) and \( m_z = 1 \)


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As an example, let us assume that the $E_z$ update equation in (5) is used for an FV24 cell in close proximity to the TFSF interface such that $E_z$ and most of the $H$ terms in the right hand side are within the scattered field region, except for the $H_z$ terms at the $J−(3/2)$ offset from $E_z$’s $J$ position. In this case, the $H_z$ terms in question contain total field information and need to be modified by subtracting source information from them. This is effected by executing the following correction equation after (5) for this particular FV24 cell

\[
E_{\nu J,K} = E_{\nu J,K}^{\text{old}} - \alpha H_{\nu J,K}^{\text{old}} - \beta H_{\nu J,K}^{\text{old}}
\]

where all the $H^\mu$ terms are strictly source values mapped from the 1D propagator.

### Table 1
Indices for some field locations from the FV24 $E_z$ update equation

<table>
<thead>
<tr>
<th>Field Location</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{\nu J,K}$</td>
<td>$\frac{j}{3m_x - 1}$</td>
</tr>
<tr>
<td>$H_{\nu J,K}$</td>
<td>$\frac{j + m_x}{2} - \frac{1}{2} + m_y$</td>
</tr>
<tr>
<td>$H_{\nu J,K}$</td>
<td>$\frac{j + m_x}{2}$</td>
</tr>
<tr>
<td>$H_{\nu J,K}$</td>
<td>$\frac{j - m_y}{2}$</td>
</tr>
</tbody>
</table>

### 4 Waveform initiation within the 1D propagator

To initiate a waveform on the 1D grid, the first few nodes therein need to be hard wired at every time step using either analytical expressions (analytic source method) or the optimised analytic field propagator (O-AFP) [14, 15]. The extent of the propagator nodes requiring this treatment depends on the selection of ($m_x$, $m_y$, $m_z$) which widens the effective FV24 cell reach as these integers grow. Both approaches require the numerical wavenumber $k$ which is obtained by solving the FV24 dispersion relation [1]

\[
\left( \frac{c}{\Delta t} \right)^2 \sin \left( \frac{\omega \Delta t}{2} \right) = K_x \sin \left( \frac{k_x}{2} \right) + \frac{1}{3} \sin \left( \frac{3k}{2} h/2 \right)
\]

where

\[
K_x = K_x + K_x \left( \cos \left( \frac{k_x}{2} \right) + \cos \left( \frac{k_x}{2} \right) \right) + K_x \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_x}{2} \right)
\]

Choosing the O-AFP approach and given an appropriately band-limited time series $f(t)$ at a reference point on the 1D
grid, the numerical wavenumber \( \vec{k} \) is used to delay \( f^i_{\text{ref}} \) and find the incident field time series \( f^0_{\text{ref}} \) at those few initial nodes

\[
f^0_{\text{ref}}(t) = \text{FFT}^{-1}\left( \text{FFT}\left[f^i_{\text{ref}}(t)\right] e^{-i\vec{k}_0 \cdot \vec{x}} \right)
\]

(8)

\[
f^0_{\text{ref}}(t) = \frac{1}{\eta} \text{Re}\left[ \text{FFT}^{-1}\left( \text{FFT}\left[f^i_{\text{ref}}(t)\right] e^{-i\vec{k}_0 \cdot \vec{x}} \right) \right],
\]

(9)

where \( \vec{k}_0 \) is based on the pulse’s centre frequency. A discussion of the choice of number of points used for FFT and inverse FFT is presented in [15, 16]. Once these time series are obtained, electromagnetic field components \((E_{\text{i},1,2,3} \text{ and } H_{\text{i},1,2,3})\) can be expressed using the appropriate polarisation projections

\[
E^o_{\text{i},1,2,3} = f^0_{\text{ref}}(t)
\]

\[
E^o_{\text{i},1,2,3} = f^0_{\text{ref}}(t) (\cos \psi \sin \tilde{\phi} - \sin \psi \cos \tilde{\phi} \cos \tilde{\theta})
\]

(10)

\[
E^o_{\text{i},1,2,3} = f^0_{\text{ref}}(t) (\cos \psi \sin \tilde{\phi} - \sin \psi \cos \tilde{\phi} \sin \tilde{\theta})
\]

(11)

\[
E^o_{\text{i},1,2,3} = f^0_{\text{ref}}(t) (\sin \psi \sin \tilde{\phi} \cos \tilde{\theta} + \cos \psi \cos \tilde{\phi} \sin \tilde{\theta})
\]

(12)

\[
H^o_{\text{i},1,2,3} = f^0_{\text{ref}}(t) (\cos \psi \sin \tilde{\phi} \cos \tilde{\theta} + \sin \psi \cos \tilde{\phi} \sin \tilde{\theta})
\]

(13)

\[
H^o_{\text{i},1,2,3} = f^0_{\text{ref}}(t) (\sin \psi \sin \tilde{\phi} \cos \tilde{\theta} - \cos \psi \cos \tilde{\phi} \sin \tilde{\theta})
\]

where \( \psi \) is the nominal angle the vector \( E \) makes with \( \hat{x} \times \hat{P} \) [15] (a user input parameter). The numerically rendered polarisation angles are given by

\[
\tan \tilde{\phi} = \frac{\tilde{P}_y}{\tilde{P}_x}, \quad \tan ^2 \tilde{\theta} = \frac{\tilde{P}_y^2 + \tilde{P}_z^2}{\tilde{P}_x^2},
\]

(14)

where \( \tilde{P}^2_{x,y,z} \) are obtained from the right hand side of (7) after solving for \( \tilde{k} \).

5 Numerical results

The above TFSF method for exciting a plane wave in an FV24 grid is implemented with no scatterers inside the total field region. Consequently, any measured electromagnetic fields in the scattered field region will be purely due to imperfections in the used TFSF technique. The waveform used is the modulated Gaussian pulse

\[
f^i_{\text{ref}} = \cos \left( \omega_0 (\Delta t - n_0) \right) e^{-\left( (\Delta t - n_0) / \sigma \right)^2}.
\]

(15)

For a distortion free pulse propagation, \( n_0 = 2\sqrt{2.3/\pi} \Delta f \) and \( n_0 = 4.5n_0 \), are chosen [7] where \( \Delta f \) is the range of frequencies of the Gaussian pulse spectrum around the carrier frequency with an amplitude exceeding 10% of pulse maximum. Other simulation parameters include 2 GHz carrier frequency, a uniform 20 cells per wavelength grid resolution at 1 GHz, maximum FV24 time step \( \Delta t = \frac{h}{c/\sqrt{3}} \frac{3}{|3 - 4k_y - 2k_z - 4k_d|} \).

(16)

a total field region size of \( 40 \times 40 \times 40 \) cubic cells, rational angle integers \((m_x, m_y, m_z) = (0, 3, 13)\), and wave polarisation \( \phi = \pi/3 \). Fields are observed after the simulation advances 300 time steps.

Fig. 5 shows the modulated Gaussian pulse within the 1D propagator, while Fig. 6 shows the corresponding mapped plane wave onto the main grid. As expected, no fields are present within the scattered field region due to the absence of a scatterer. To
isolate any potential field leakage into the scattered field region due to TFSF residual errors, Fig. 6 is replotted in Fig. 7 after the total field region values are set to zero. As expected, no field leakage there exceeds the $-300 \text{ dB} (10^{-15})$ noise floor caused by the computing platform truncation error. All other electromagnetic field components exhibit the same precision and accuracy.

6 Conclusion

Application of the excellent 1D MAP TFSF technique for initiating plane wave sources within the high-order extended-stencil FV24 algorithm has been developed. The 1D propagator design and custom update equations are presented. Field mapping from the auxiliary 1D propagator to the main FV24 grid is graphically illustrated. The process of initiating a plane wave on the 1D propagator using proper phase delays is outlined. Spurious field leakages are demonstrated to be upper bound by the underlying computing platform finite-word truncation errors. The developed technique expands the FV24 modelling capabilities to include analysis and characterisation of electrically large scattering structures.

7 References