Extracting Field Information Embedded Within a Coarse Pseudospectral Time-Domain Simulation

Jake W. Liu, Yueh-Sheng Hsu, and Snow H. Tseng

***Abstract*—With a coarse simulation grid, the pseudospectral time-domain (PSTD) simulation technique is advantageous to model macroscopic electromagnetic problems or optics problems. Due to the coarse grid appearance, the high accuracy and fine details of the field distribution in a PSTD simulation are often overlooked and underestimated. Here, we propose a numerical technique to harness the embedded field information as dictated by the Nyquist limit. Simulation results show that the proposed densification technique can be applied to 1-D, 2-D, or 3-D PSTD simulations and reconstruct the coarse grid into a high-resolution field distribution, revealing fine field variations that were not visible before.**

***Index Terms*—Densification, pseudospectral time-domain method (PSTD), sampling theorem.**

I. Introduction

THE pseudospectral time-domain (PSTD) technique, first proposed by Liu [1], is a simulation technique beneficial for modeling large-scale problems. Trigonometric functions, Legendre polynomials, or Chebyshev polynomials are employed to approximate the spatial derivatives; the PSTD technique is a variant of the widely used finite-difference time-domain (FDTD) simulation technique in computational electrodynamics [2]. Recently, new variations of the PSTD algorithm have been reported [3]. In addition to electromagnetics, it is also applicable to elastic and acoustic wave propagation and other time-dependent problems [4]–[6]. With its advantage to handle large-scale simulations, the PSTD technique can be applied to a wide range of problems.

The PSTD technique utilizes information of the entire domain to approximate the derivatives of any given point. Gibbs phenomenon emerges due to discontinuities in the PSTD simulation; various efforts to tackle this problem have been reported [7]–[10]. Compared to the FDTD technique, PSTD utilizes fewer grid points to achieve a high accuracy; since the wavelength is generally much smaller than the size of scatterers, the PSTD technique is advantageous over FDTD that requires a very fine grid in modeling large-scale optics problems [11].

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The research objective is to exploit the spectral accuracy of the PSTD algorithm and extract field information embedded within a coarse PSTD grid. In contrast to the second-order FDTD simulation, which uses only adjacent grid points to approximate the derivatives, the PSTD simulation utilizes information of all grid points in the entire computational domain to approximate the spatial derivatives, thus achieving higher accuracy than the FDTD algorithm. In this letter, we report a postprocessing technique for high-order numerical algorithms (e.g., the PSTD simulation) that can refine the spatial distribution to reconstruct a high-resolution field distribution, as allowed by the sampling theorem (Nyquist limit) [12].

II. Formulation

Here, we introduce the fundamentals of the Fourier PSTD algorithm, followed by the proposed densification technique. The formulation of PSTD is briefly introduced in Section II-A; the densification technique is described in Section II-B.

A. PSTD Simulation

The PSTD technique is a time-domain technique for approximating partial differential equations that are typically implemented on a collocated spatial grid. To illustrate the PSTD algorithm, we consider a general field component ψ, of which the spatial derivatives in the η direction at any grid point j can be computed by

$$\partial_\eta \psi|_j \approx F_\eta^{-1}\left[ik_\eta F_\eta(\psi)\right]\big|_j, \quad \eta := x, y, z \tag{1}$$

where k_η is the wavenumber, and F_η and F_η^{-1} are the discrete Fourier transform (DFT) and the inverse discrete Fourier transform (IDFT) along the η direction, respectively. Here, we present an example of a one-dimensional (1-D) PSTD simulation; the total extent of the simulation space is L: $\eta \in [0, L)$, the uniformly spaced cell size is $\Delta\eta = L/N$, and N is the total number of samples in the η-axis. The spatial derivative can be expanded as

$$\partial_\eta \psi|_j \approx \frac{1}{N}\sum_{m=-N/2}^{N/2-1} ik_m \hat{\psi}(m)\, e^{ik_m \eta_j} \tag{2}$$

with $k_m = 2\pi m/L$, $\eta_j = j\Delta\eta$ the jth grid position, and $m = 0, 1, \ldots, N-1$. The Fourier series is given by

$$\hat{\psi}(m) = \sum_{j=0}^{N-1} \psi(\eta_j)\, e^{-ik_m \eta_j}. \tag{3}$$

Notice that (2) and (3) can be computed via the fast Fourier transform (FFT) algorithm, and the total operation can be reduced to $0.5N \log_2 N$ [13].

B. Densification Technique

In order to recover the field information embedded within a coarse PSTD grid, we analyze the PSTD simulation with the sampling theorem concept proposed by Nyquist [14] and Shannon [12]. Unlike FDTD, the PSTD algorithm exploits spectral properties of a function to approximate differentiation; all the field information is used to approximate the partial derivatives, approaching the Nyquist limit of recovering the time-domain signal with two points per wavelength. With a coarse grid, the PSTD simulation achieves similar or better accuracy as a fine-grid FDTD simulation.

For high-order algorithms such as the PSTD algorithm, the embedded information of the field is not apparent in a coarse grid; a high-resolution grid is required to reveal field information contained in the coarse PSTD grid. According to [12], the field values between the grid points can be accurately acquired by convolution with a sinc function

$$\frac{\sin\left(2\pi W\eta\right)}{2\pi W\eta} \tag{4}$$

where $W = N/2L$ is the approximated bandwidth in the spatial domain. Thus, the field over the domain can be reconstructed by

$$\psi(x,y,z) = \sum_{j=0}^{N_x-1}\sum_{l=0}^{N_y-1}\sum_{m=0}^{N_z-1}\left[\psi\left(x_j,y_l,z_m\right)\cdot\frac{\sin\pi\left(2W_x x-j\right)}{\pi\left(2W_x x-j\right)}\cdot\frac{\sin\pi\left(2W_y y-l\right)}{\pi\left(2W_y y-l\right)}\cdot\frac{\sin\pi\left(2W_z z-m\right)}{\pi\left(2W_z z-m\right)}\right] \tag{5}$$

where x_j, y_l, z_m are the sample points, and W_x, W_y, W_z are the approximated bandwidths in the *x*-, *y*,- and *z*-directions, respectively. Though only discrete grid points are present in the simulation, the field values at arbitrary spatial positions can be acquired from the coarse sample values. A high-resolution field distribution can be reconstructed via convolution with a sinc function to reveal the fine details of the field distribution that were not shown in the coarse PSTD grid. Essentially, the proposed densification technique enables modeling a problem with a coarse PSTD grid, yet achieving resolution and accuracy of a fine, high-resolution FDTD simulation.

The resolution of the reconstructed grid can be increased by adding more points between grid points. However, the field details revealed by the densification technique are not unlimited—the information that can be extracted is only as much as is contained in the PSTD grid, as dictated by the Nyquist limit. The densification technique is not applicable to low-order simulations such as the second-order FDTD simulation; it is suitable for high-order numerical schemes such as the PSTD algorithm where field information is embedded in the coarse grid that is not readily visible.

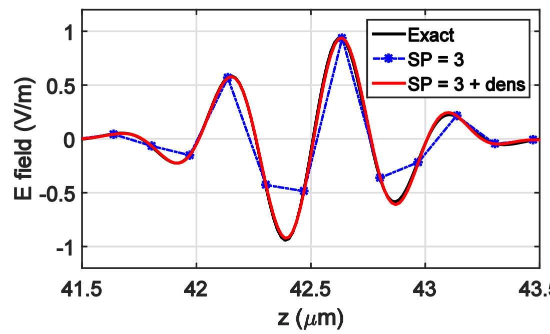

Fig. 1. 1-D PSTD simulation of a sinusoidal pulse. The sinusoidal wave is modulated by a Gaussian pulse (6). Black line: Analytical solution of a propagating 600 THz Gaussian sine pulse. Blue dash-dot line: PSTD simulation with a resolution of three grid points per wavelength. Red line: PSTD with densification.

III. Numerical Results

We employ the proposed densification technique to 1-D, 2-D, and 3-D PSTD simulation of various wave propagation problems. The accuracy of the PSTD simulation is easily underestimated by its coarse appearance; here, we demonstrate reconstructing the coarse PSTD grid into a high-resolution field distribution. An error analysis is shown to quantify the performance of the densification technique.

A. 1-D PSTD Simulation

We employ the densification technique to a 1-D PSTD simulation. Due to the DFT involved in the PSTD algorithm, abrupt variations of the field need to be smoothened to avoid causing numerical artifacts. A 1-D PSTD simulation of a sinusoidal wave modulated by a Gaussian pulse (6) is presented in Fig. 1; the Gaussian envelope is used to taper down the field to avoid exciting high-frequency numerical artifacts

$$E\left(x\right) = \exp\left(\left(\frac{x}{\lambda}\right)^2\right)\sin\left(\frac{2\pi x}{\lambda}\right). \tag{6}$$

The frequency of the sine wave is 600 THz (wavelength $\lambda = 0.5\ \mu$m), time step *dt* is 10^{-2}fs, and the spatial resolution *dx* is 0.16667 μm (three sample points per wavelength).

As shown in Fig. 1, the PSTD simulated pulse is compared to the exact solution (black line). Notice that the PSTD simulated pulse is a coarse approximation of the exact solution. Judging by the blue curve, the PSTD simulated pulse appears to be rough and hardly resembles the exact solution. Nevertheless, the seemingly coarse PSTD grid is actually very accurate and contains a lot of information than its appearance. By applying the proposed densification technique, the embedded field information can be extracted to reconstruct the coarse PSTD simulated pulse (blue dash-dot line) into a fine smooth pulse (red line) that matches the exact solution. It is clear that the PSTD simulation with densification (red line) is nearly a perfect match of the exact solution, as shown in Fig. 1.

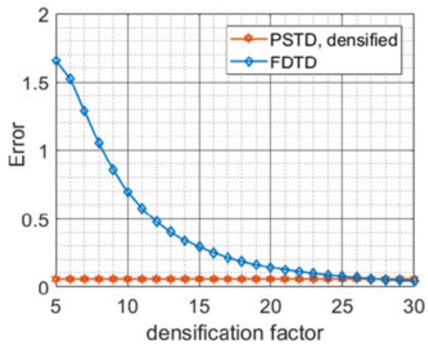

Fig. 2. Error analysis of the PSTD with densification compared to FDTD. Both FDTD and PSTD with densification are compared with the same grid resolution. A high-resolution FDTD grid is required to achieve comparable accuracy as the PSTD simulation with densification.

To quantify the accuracy of the reconstructed field via densification, we calculate the 2-norm of E by

$$\|E\|_2 = \sqrt{\sum_{j=0}^{N-1} E_j^2} \tag{7}$$

where N is the total length of the simulation domain. The error is calculated by

$$\text{Error} = \frac{\|E_{\text{num}} - E_{\text{exact}}\|_2}{E_{\|\text{exact}\|_2}} \tag{8}$$

where E_{num} is the numerical solution, and E_{exact} is the exact solution.

As a reference, the PSTD after densification is compared to an FDTD simulation of the same grid resolution. The error versus the densification factor is shown in Fig. 2; the densification factor is defined as the ratio of the resolution of the densified grid to the original coarse PSTD grid. Since the FDTD method is based upon a difference scheme to approximate the derivatives, the error of the FDTD simulation decreases with the increase of grid resolution (see Fig. 2). Unlike common interpolation methods, the densification method extracts information contained in the grid, and the reconstructed field is highly accurate; as shown in Fig. 3, the error remains to be a constant value of 0.0567. The oscillatory behavior known as Runge's phenomenon can account for the constant error [5]. Notice that for an FDTD simulation to achieve comparable accuracy as the PSTD simulation with densification, a grid resolution of 84 FDTD grid points per wavelength is required.

Furthermore, we compare the proposed method with commonly used interpolation methods, e.g., linear and cubic spline interpolation [15]. Unlike these interpolation methods, which match the existing data to a pregiven function, the proposed densification technique exhibits outstanding accuracy as it exploits the sampling theorem and reconstructs the missing data points exactly with information embedded within the simulation grid, allowed by the Nyquist limit [14]. By calculating the RMS error of simulating a sinusoidal wave modulated by a Gaussian pulse (6), the performance of the proposed densification technique is compared to linear interpolation and spline interpolation; the proposed densification technique exhibits superior accuracy (error $= 0.0032$) over linear interpolation (error $=$ 0.1478) or cubic spline (error $= 0.0248$).

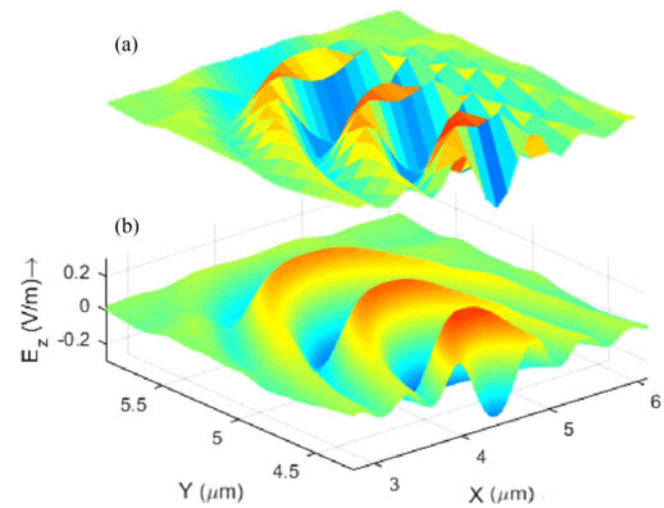

Fig. 3. 2-D PSTD simulation of a single-slit diffraction. A 600 THz sinusoidal plane wave is diffracted by a single slit (width is one wavelength). The simulation grid resolution is four grid points per wavelength. (a) Original coarse PSTD simulation. (b) PSTD simulation with densification.

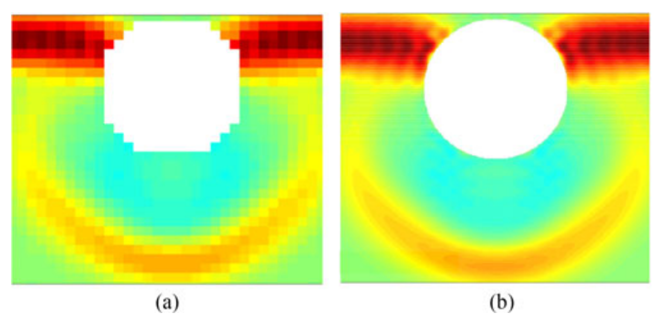

Fig. 4. 2-D PSTD simulation of the transient phenomenon of a TE Gaussian plane wave backscattered by a perfect conducting cylinder. (a) Original PSTD grid. (b) After densification, the reconstructed field distribution reveals fine details. Radius of the cylinder is 0.625 μm; grid size is 0.083 μm.

B. 2-D PSTD Simulation

As shown in Fig. 3, the densification technique is applied to a 2-D PSTD simulation of the single-slit diffraction phenomenon. A coarse PSTD grid of four grid points per wavelength is employed. After densification, the coarse PSTD grid is reconstructed into a high-resolution field distribution, as shown in Fig. 3(b). By comparing Fig. 3(a) and (b), it is clear that fine details of the field variation (e.g., wave troughs) are recovered via densification, which cannot be accomplished by simple interpolation.

With the proposed densification technique, accurate field information of arbitrary position can be acquired. In Fig. 4, we model the diffraction of a plane wave impinging upon a conducting cylinder [16], [17]—a TE Gaussian plane wave propagates in the $+y$-direction and is diffracted by the cylinder. We analyze the backscattered field and the phenomenon of transient

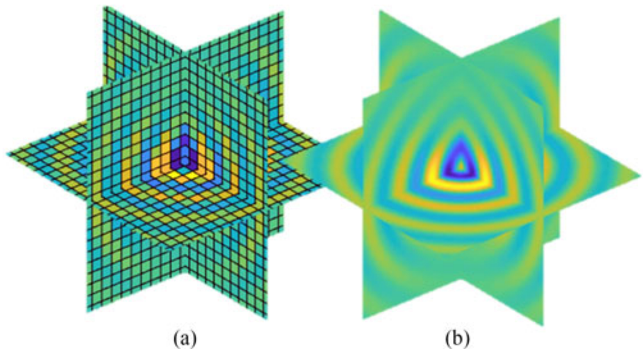

Fig. 5. 3-D PSTD simulation of a sinusoidal current source J_z. The sinusoidal current oscillates $J_z = \sin(2\pi fct)$ with a frequency of $f_c = 1500\,\text{THz}$. A cubic region of 1 μm^3 is simulated with a resolution of 62.5 nm. (a) Original PSTD simulation with a resolution of 3.2 grid points per wavelength. (b) PSTD simulation with densification (densification factor = 5).

electromagnetic scattering. The Gaussian pulse is given by

$$g(t) = \exp\left(-(t-t_0)^2/\tau^2\right) \quad (9)$$

where τ is the duration of the pulse $(2f_c)^{-1} = (2 \times 6 \times 10^{14})^{-1} = 8.\bar{3} \times 10^{-16}$ s, and $t_0 = 3\tau$ is the time shift. A cylinder with a radius of $2.5 \times c_0 \times \tau \approx 0.6246\,\mu$m is placed at the center of the simulation space. As shown in Fig. 4(a), the 2-D PSTD simulation is implemented with a coarse grid resolution of six grid points per wavelength; discretization due to the grid coarseness is pronounced. After applying the proposed densification technique, the coarse simulation is reconstructed into a high-definition field variation revealing fine details [see Fig. 4(b)], consistent with the results of [17]. It is clear that the proposed densification technique brings out accurate field information that is embedded in the PSTD simulations.

C. 3-D PSTD Simulation

Last, we model a current source radiating in 3-D. A sinusoidal current oscillates $J_z = \sin(2\pi f_c t)$ with a frequency of $f_c = 1500\,\text{THz}$. The propagating E-field in a cubic region of 1 μm^3 is simulated. As shown in Fig. 5(a), the 3-D PSTD simulation is implemented with a coarse grid resolution of 3.2 grid points per wavelength; significant stair-casing of the field is visible. Simulations show that the proposed densification can effectively extract the embedded field information and reconstruct it into a high-resolution distribution revealing fine details that were not visible before.

IV. Conclusion

With a coarse spatial grid, the PSTD simulation achieves accuracy comparable to a high-resolution FDTD simulation; however, the high accuracy of the PSTD simulation is often underestimated by the appearance of a coarse grid. Mathematically similar to the sinc interpolation method used in digital signal processing, the densification technique is more accurate than common interpolation methods as it enables extracting field information contained in the coarse PSTD simulation to recreate a high-resolution field distribution revealing fine details that were not visible before.

Based upon exploiting the information embedded within a coarse grid, the densification technique is generally applicable to PSTD simulations of band-limited problems as well as continuous-wave problems. Together, Figs. 1 and 3–5 demonstrate the densification technique applied to 1-D, 2-D, and 3-D PSTD simulations. An error analysis presented in Section III-A shows that the proposed densification technique is far more accurate than other interpolation methods.

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