Local spectral time-domain method for electromagnetic wave propagation

Gang Bao

Department of Mathematics, Michigan State University, East Lansing, Michigan 48824

G. W. Wei

Department of Mathematics, Michigan State University, East Lansing, Michigan 48824, and Department of Computational Science, National University of Singapore, Singapore 117543

Shan Zhao

Department of Computational Science, National University of Singapore, Singapore 117543

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We explore the feasibility of using a local spectral time-domain (LSTD) method to solve Maxwell's equations that arise in optical and electromagnetic applications. The discrete singular convolution (DSC) algorithm is implemented in the LSTD method for spatial derivatives. Fourier analysis of the dispersive error of the DSC algorithm indicates that its grid density requirement for accurate simulations can be as low as approximately two grid points per wavelength. The analysis is further confirmed by numerical experiments. Our study reveals that the LSTD method has the potential to yield high resolution for solving large-scale electromagnetic problems. © 2003 Optical Society of America

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Time-dependent electromagnetic problems are solved mainly by either global or local methods. Global methods, such as pseudospectral time-domain methods,[1,2] are usually highly accurate. But local methods, such as finite-difference time-domain methods,[3] are much more flexible for handling complex boundaries and geometries. For large-scale electromagnetic problems, which involve as many as thousands of wavelengths in complex domains, there is a clear need for developing innovative numerical methods that would have the accuracy of global methods and the flexibility of local methods. To this end, numerous highly accurate approaches have been reported in the literature, including various higher-order finite-difference (FD) schemes[4–7] and a multiresolution time-domain method.[8,9] Because they are able to produce much smaller approximation errors, these schemes found their success in modeling electromagnetic waves.

Our objective in this Letter is to introduce a local spectral time-domain (LSTD) method for solving large-scale electromagnetic problems. Our basic approach is to use the discrete singular convolution (DSC) algorithm[10] that has been proposed as a potential numerical method for solving many computational problems. The DSC algorithm has been shown to have spectral convergence,[11] and it has been used for treating some complex boundary conditions.[12] The unified feature of the DSC formalism has been discussed in Ref. 13. A comprehensive comparison of the Fourier pseudospectral and DSC methods has been made for solution of partial differential equations.[14]

Assuming the absence of charge density and current sources, and linear isotropic constitutive relations, we find that the transverse magnetic modes are governed by the following time-dependent two-dimensional Maxwell equations:

$$\mu \frac{\partial D_z}{\partial t} = \frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y},$$

$$\epsilon \frac{\partial B_x}{\partial t} = -\frac{\partial D_z}{\partial y}, \qquad \epsilon \frac{\partial B_y}{\partial t} = \frac{\partial D_z}{\partial x}, \tag{1}$$

where D and B are, respectively, the electric and the magnetic flux densities and ϵ and μ are the electric permittivity and the magnetic permeability of material, respectively, and are piecewise constant. Throughout, the medium is assumed to be nonmagnetic with $\mu = 1$.

For the LSTD method, a function and its nth-order derivative are approximated by means of a discretized convolution:

$$f^{(n)}(x) \approx \sum_{k=-M}^{M} \delta_{\alpha,\sigma}^{(n)}(x - x_k) f(x_k), \qquad n = 0, 1, \ldots, \tag{2}$$

where $2M + 1$ is the computational bandwidth and $\delta_{\alpha,\sigma}(x - x_k)$ denotes the (regularized) DSC kernel, where $\delta_{\alpha,\sigma}^{(n)}(x - x_k) = d^n \delta_{\alpha,\sigma}(x - x_k)/dx^n$ is its higher-order derivative terms.[10] The regularized Shannon kernel (RSK),[10]

$$\delta_{h,\sigma}(x - x_k) = \frac{\sin[(x - x_k)\pi/h]}{(x - x_k)\pi/h} \exp\left[-\frac{(x - x_k)^2}{2\sigma^2}\right],$$

is employed in the present LSTD method, where h is the grid spacing. Parameter σ in the RSK often varies in association with h, i.e., $\sigma = rh$, where r is a parameter chosen in computation. It was recently proved that the truncation error of the RSK decays exponentially with respect to the increase in sampling points.[11]

The dispersive errors of the central difference and DSC schemes are illustrated in Fig. 1. It is evident

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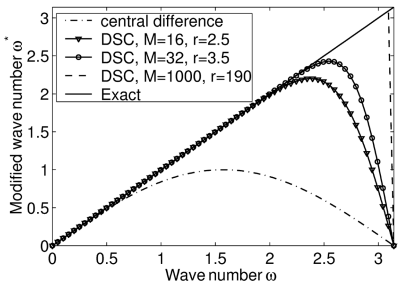

Fig. 1. Plots of the dispersion errors.

that the DSC approximations remain close to the exact differentiation until a high wave number is reached, whereas the second-order central difference deviates from the exact value at much lower wave numbers. Moreover, as M gets larger in the RSK, the dispersive error becomes smaller. It is well known that pseudospectral methods can provide highly accurate derivative approximations by using a grid density (GD) of two grid points per wavelength (PPW). The GD requirement of the DSC algorithm for accurate modeling can also be chosen to be close to 2 PPW when M is sufficiently large. For example, the RSK derivative approximation with $M = 1000$ and $r = 190$ (Fig. 1) is almost exact, except when $\omega = \pi$, i.e., sampling at the Nyquist limit. Therefore the DSC algorithm is well suited for accurate computation of large-scale electromagnetic problems. The rest of this Letter is devoted to two numerical tests. Similarly to the FDTD method, a staggered grid system is used in the LSTD method.

To explore the potential of the DSC algorithm for electromagnetic simulations, we first consider a scattering problem of a dielectric square.[7] As shown in Fig. 2, the dielectric material ($\epsilon = 4$) in the center of the domain is surrounded by air ($\epsilon = 1$). A Gaussian pulse, $E_z(x, y, t) = \exp\{-[x\cos(\pi/4) + y\sin(\pi/4) + 1/2 - t]^2/(2 \times 0.03^2)\}$, is incident upon the dielectric square at an angle $\pi/4$. Following Ref. 7, the incident field is imposed along the entire outer boundary, and spurious reflections at boundaries are not considered. For comparison, both the second-order FD (FD2) and the fourth-order FD (FD4) centered schemes are also employed. In all schemes, a uniform grid with $h = \Delta x = \Delta y$ is employed, and the fourth-order Runge–Kutta method with a sufficiently small time increment $\Delta t = 0.0005$ is used. For the LSTD method, we choose $M = 8$ with $r = 1.9$. To account for the discontinuity in the electric flux density, a simple ϵ-smoothing technique[6] that replaces the discontinuous permittivity function ϵ with a fourth-order approximation is utilized in both the FD4 scheme and the LSTD. The resultant approximation errors at $t = 1.4$ are depicted in Fig. 3. It is clear that the errors in the FD4 scheme and the DSC are significantly smaller than that of the FD2 scheme, even when a coarser grid is employed. Moreover, Fig. 4 shows that the DSC error is smaller than that of the FD4 scheme, especially inside the dielectric.

We next consider a benchmark waveguide problem to explore the potential use of the LSTD method for large-scale electromagnetic computation. Consider a two-dimensional air-filled square waveguide ($\epsilon = 1$) of size $a \times a$. The initial electric field is given by $E_z(x, y, 0) = \sin(n\pi x/a)\sin(n\pi y/a)$. For simplicity, we set $a = 2n\pi$. The fact that this problem admits of a time-dependent analytical solution $E_z(x, y, t) = E_z(x, y, 0)\cos(2^{1/2}t/2)$ allows us to validate the LSTD method objectively. A uniform mesh with mesh size $N \times N$ is used with a GD of $2N/n$ PPW. An image principle[9] is used to model the electric and magnetic walls. To study large-scale problems we choose a low-storage Runge–Kutta method[15] for the time integration. A middle-sized study with $n = 200$ and $M = 200$ is considered first. It can be observed from Table 1 that extremely accurate results can be obtained from the LSTD method when the GD is as

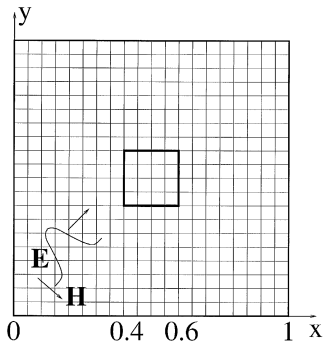

Fig. 2. Geometry of the dielectric square problem.

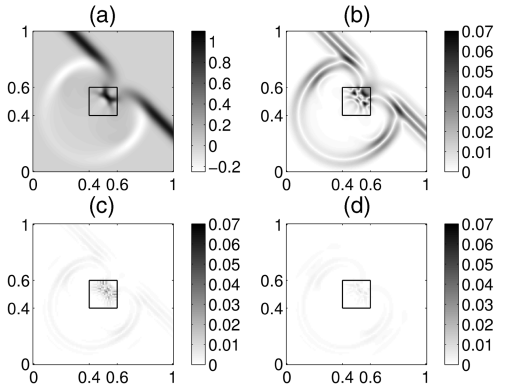

Fig. 3. Contour plots of an electric field and errors in the electric field. (a) Reference solution generated by use of the DSC algorithm with $h = 0.0025$, (b) FD2 error ($h = 0.005$), (c) FD4 error ($h = 0.01$), (d) DSC error ($h = 0.01$). Because the errors are small, the gray scales for the errors have much shorter ranges than that of the reference solution.

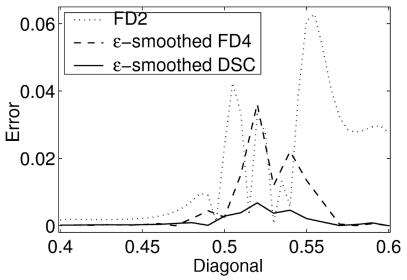

Fig. 4. Absolute errors in the electric field across the diagonal of a dielectric square.

Table 1. Numerical Errors of the LSTD Method with $M = 200$ and $n^2 = 200^2$[a]

				$t = 5.0$		$t = 10.0$	
N^2	GD	Kernel	r	L_∞	L_2	L_∞	L_2
202^2	2.02	RSK	1000	1.68(−4)	8.34(−5)	6.19(−4)	3.08(−4)
		SK		1.67(−4)	8.32(−5)	6.18(−4)	3.07(−4)
210^2	2.10	RSK	40.4	6.16(−9)	3.06(−9)	2.27(−8)	1.13(−8)
		SK		5.06(−5)	2.52(−5)	1.87(−4)	9.29(−5)
220^2	2.20	RSK	27.7	1.40(−14)	2.38(−15)	7.54(−14)	2.81(−14)
		SK		2.44(−5)	1.21(−5)	9.05(−5)	4.50(−5)

[a]Small time increments are used: $\Delta t = 0.1, 0.025, 0.001$ for $N = 202, 210, 220$, respectively. Here 1.68(−4) denotes 1.68×10^{-4}.

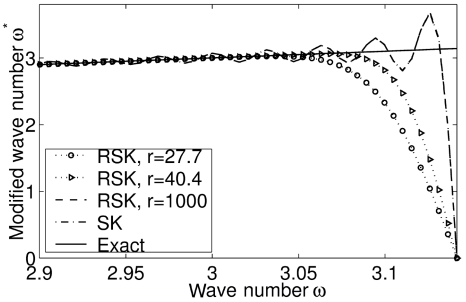

Fig. 5. Plot of dispersive errors with $M = 200$.

Table 2. Large-Scale Electromagnetic Study[a]

N^2	n^2	Δt	r	L_∞	L_2
2020^2	2000^2	5.0(−3)	190.0	5.69(−13)	2.84(−13)
4040^2	4000^2	1.0(−2)	187.5	6.96(−14)	3.44(−14)
8080^2	8000^2	1.25(−2)	187.0	2.16(−13)	1.08(−13)

[a]$t = 0.1$; $M = 1000$; GD, 2.02 PPW; optimized r.

small as 2.2 PPW. However, when one pushes the GD toward 2 PPW, the accuracy decreases. Previous Fourier analysis suggests that this is so because the dispersive error of the antisymmetric kernel attains its maximum value of π at the Nyquist limit. Nevertheless, the LSTD approximation with GD = 2.02 PPW can still be optimized through r. As can be observed from Fig. 5, as r increases, the RSK approximation remains close to the exact differentiation up to larger wave numbers, even though strong oscillations occur. In fact, as $r \to \infty$, the RSK degenerates to the Shannon kernel (SK)

$$\delta_{h,\sigma}(x - x_k) = \frac{\sin[(x - x_k)\pi/h]}{(x - x_k)\pi/h}.$$

It can be seen from Fig. 5 that the dispersive error of the SK is almost identical to that of the RSK with $r = 1000$ and that such global dispersive error is actually the smallest one. Consequently, similar results are obtained by use of both kernels when the GD is 2.02 PPW (Table 1). Note that such accuracy is beyond the capability of the (higher-order) finite-difference time-domain methods. Therefore, although the Nyquist sampling limit is generally not recommended for the DSC algorithm, high accuracy can be obtained if the GD is slightly larger than 2 PPW. We finally consider several large-scale computation cases that are intractable when conventional finite-difference time-domain methods are used. As indicated in Table 2, extremely accurate results are obtained with only 2.02 PPW for these challenging problems.

In summary, we have explored the utility of a local spectral method, the DSC algorithm, for solving large-scale electromagnetic problems. By means of discrete Fourier analysis, the dispersive error of the DSC algorithm was investigated. Several numerical experiments were carried out to illustrate the high accuracy of the DSC algorithm for practical electromagnetic applications. Our present study indicates that the DSC algorithm is accurate, flexible, and efficient for large-scale electromagnetic computations.

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References

1. T. A. Driscoll and B. Fornberg, J. Comput. Phys. **140,** 47 (1998).
2. Q. H. Liu, IEEE Trans. Geosci. Remote Sens. **37,** 917 (1999).
3. K. S. Yee, IEEE Trans. Antennas Propag. **AP-14,** 302 (1966).
4. Z. Haras and S. Ta'asan, J. Comput. Phys. **114,** 265 (1994).
5. J. B. Cole, Comput. Phys. **11,** 287 (1997).
6. E. Turkel, in *Advances in Computational Electrodynamics: The Finite-Difference Time-Domain Method*, A. Taflove, ed. (Artech House, Boston, Mass., 1998), Chap. 2.
7. H. M. Jurgens and D. W. Zingg, SIAM J. Sci. Comput. **22,** 1675 (2000).
8. M. Krumpholz and J. Oliger, IEEE Trans. Microwave Theory Tech. **44,** 555 (1996).
9. L. P. B. Katehi, J. F. Harvey, and E. Tentzeris, in *Advances in Computational Electrodynamics: The Finite-Difference Time-Domain Method*, A. Taflove, ed. (Artech House, Boston, Mass., 1998), Chap. 3.
10. G. W. Wei, J. Chem. Phys. **110,** 8930 (1999).
11. G. Bao, G. W. Wei, and A. H. Zhou, "Analysis of regularized Whittaker–Kotel'nikov–Shannon sampling expansion" submitted to SIAM J. Numer. Anal.
12. G. W. Wei, Y. B. Zhao, and Y. Xiang, Int. J. Numer. Meth. Eng. **55,** 913 (2002).
13. G. W. Wei, J. Phys. A **33,** 4935 (2000).
14. S. Y. Yang, Y. C. Zhou, and G. W. Wei, Comput. Phys. Commun. **143,** 113 (2002).
15. D. W. Zingg and T. T. Chisholm, Appl. Numer. Math. **31,** 227 (1999).