A Spectral Time-Domain Method for Computational Electrodynamics

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Abstract. Ever since its introduction by Kane Yee over forty years ago, the finite-difference time-domain (FDTD) method has been a widely-used technique for solving the time-dependent Maxwell's equations. This paper presents an alternative approach to these equations in the case of spatially-varying electric permittivity and/or magnetic permeability, based on Krylov subspace spectral (KSS) methods. KSS methods for scalar equations compute each Fourier coefficient of the solution using techniques developed by Gene Golub and Gérard Meurant for approximating elements of functions of matrices by Gaussian quadrature in the spectral, rather than physical, domain. We show how they can be generalized to coupled systems of equations, such as Maxwell's equations, by choosing appropriate basis functions that, while induced by this coupling, still allow efficient and robust computation of the Fourier coefficients of each spatial component of the electric and magnetic fields. We also discuss the implementation of appropriate boundary conditions for simulation on infinite computational domains, and how discontinuous coefficients can be handled.

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INTRODUCTION

We consider Maxwell's equation on the rectangle $[0,2\pi]^3$, with periodic boundary conditions. Assuming nonconductive material with no losses, we have

$$\operatorname{div}\hat{\mathbf{E}} = 0, \quad \operatorname{div}\hat{\mathbf{H}} = 0, \quad \operatorname{curl}\hat{\mathbf{E}} = -\mu\frac{\partial\hat{\mathbf{H}}}{\partial t}, \quad \operatorname{curl}\hat{\mathbf{H}} = \varepsilon\frac{\partial\hat{\mathbf{E}}}{\partial t}, \tag{1}$$

where $\hat{\mathbf{E}}$, $\hat{\mathbf{H}}$ are the vectors of the electric and magnetic fields, and ε, μ are the electric permittivity and magnetic permeability, respectively. We assume that these two functions are smoothly varying in space.

By taking the curl of both sides of (1), we decouple the vector fields $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$ and obtain the equations

$$\mu\varepsilon\frac{\partial^2\hat{\mathbf{E}}}{\partial t^2} = \Delta\hat{\mathbf{E}} + \mu^{-1}\operatorname{curl}\hat{\mathbf{E}}\times\nabla\mu, \quad \mu\varepsilon\frac{\partial^2\hat{\mathbf{H}}}{\partial t^2} = \Delta\hat{\mathbf{H}} + \varepsilon^{-1}\operatorname{curl}\hat{\mathbf{H}}\times\nabla\varepsilon. \tag{2}$$

In his 1966 paper [1], Yee proposed the original finite-difference time-domain method for solving the equations (1). This method uses a staggered grid to avoid solving simultaneous equations for $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$, and also removes numerical dissipation. However, because it is an explicit finite-difference scheme, its time step is constrained by the CFL condition. Nonetheless, it remains a widely used method to this day, and has inspired a host of related methods, see for example [2, 3, 4].

In [5] a class of methods, called Krylov subspace spectral (KSS) methods, was introduced for the purpose of solving parabolic variable-coefficient PDE. These methods are based on techniques developed by Golub and Meurant in [6] for approximating elements of a function of a matrix by Gaussian quadrature in the *spectral* domain. In [7, 8], these methods were generalized to the second-orer wave equation, for which these methods have exhibited even higher-order accuracy.

It has been shown in these references that KSS methods, by employing different approximations of the solution operator for each Fourier component of the solution, achieve higher-order accuracy in time than other Krylov subspace methods (see, for example, [9]) for stiff systems of ODE, and, as shown in [8], they are also quite stable, considering that they are explicit methods. In [10, 11], the accuracy and robustness of KSS methods were enhanced using block Gaussian quadrature. It is our hope that the high-order accuracy achieved for the scalar wave equation can be extended to systems of coupled wave equations such as those described by Maxwell's equations.

KRYLOV SUBSPACE SPECTRAL METHODS

We first review KSS methods, which are easier to describe for parabolic problems. Let $S(t) = \exp[-Lt]$ represent the exact solution operator of the problem

$$u_t + Lu = 0, \quad t > 0, \tag{3}$$

$$u(x,0) = f(x), \quad 0 < x < 2\pi, \tag{4}$$

$$u(0,t) = u(2\pi,t), \quad t > 0. \tag{5}$$

The operator L is a second-order differential operator of the form

$$Lu = -(p(x)u_x)_x + q(x)u, \tag{6}$$

where $p(x)$ is a positive function and $q(x)$ is a nonnegative (but nonzero) smooth function. It follows that L is self-adjoint and positive definite.

Let $\langle \cdot, \cdot \rangle$ denote the standard inner product of functions defined on $[0, 2\pi]$,

$$\langle f(x), g(x) \rangle = \int_0^{2\pi} \overline{f(x)} g(x)\, dx. \tag{7}$$

Krylov subspace spectral methods, introduced in [5], use Gaussian quadrature on the spectral domain to compute the Fourier components of the solution. These methods are time-stepping algorithms that compute the solution at time $t_1, t_2, \ldots$, where $t_n = n\Delta t$ for some choice of Δt. Given the computed solution $\tilde{u}(x,t_n)$ at time t_n, the solution at time t_{n+1} is computed by approximating the Fourier components that would be obtained by applying the exact solution operator to $\tilde{u}(x,t_n)$,

$$\hat{u}(\omega, t_{n+1}) = \left\langle \frac{1}{\sqrt{2\pi}} e^{i\omega x}, S(\Delta t)\tilde{u}(x,t_n) \right\rangle. \tag{8}$$

Krylov subspace spectral methods approximate these components with higher-order temporal accuracy than traditional spectral methods and time-stepping schemes.

In [6] Golub and Meurant describe a method for computing quantities of the form

$$\mathbf{u}^T f(A)\mathbf{v}, \tag{9}$$

where $\mathbf{u}$ and $\mathbf{v}$ are N-vectors, A is an $N \times N$ symmetric positive definite matrix, and f is a smooth function. Our goal is to apply this method with $A = L_N$ where L_N is a spectral discretization of L, $f(\lambda) = \exp(-\lambda t)$ for some t, and the vectors $\mathbf{u}$ and $\mathbf{v}$ are derived from $\hat{\mathbf{e}}_\omega$ and $\mathbf{u}^n$, where $\hat{\mathbf{e}}_\omega$ is a discretization of $\frac{1}{\sqrt{2\pi}} e^{i\omega x}$ and $\mathbf{u}^n$ is the approximate solution at time t_n, evaluated on an N-point uniform grid.

The basic idea is as follows: since the matrix A is symmetric positive definite, it has real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N > 0$, and corresponding orthogonal eigenvectors $\mathbf{q}_j$, $j = 1, \ldots, N$. Therefore, the quantity (9) can be rewritten as

$$\mathbf{u}^T f(A)\mathbf{v} = \sum_{j=1}^{N} f(\lambda_j)\mathbf{u}^T \mathbf{q}_j \mathbf{q}_j^T \mathbf{v}. \tag{10}$$

We let $a = \lambda_N$ be the smallest eigenvalue, $b = \lambda_1$ be the largest eigenvalue, and define the measure $\alpha(\lambda)$ by

$$\alpha(\lambda) = \begin{cases} 0, & \text{if } \lambda < a \\ \sum_{j=i}^{N} \alpha_j \beta_j, & \text{if } \lambda_i \leq \lambda < \lambda_{i-1} \\ \sum_{j=1}^{N} \alpha_j \beta_j, & \text{if } b \leq \lambda \end{cases}, \quad \alpha_j = \mathbf{u}^T \mathbf{q}_j, \quad \beta_j = \mathbf{q}_j^T \mathbf{v}. \tag{11}$$

If this measure is positive and increasing, then the quantity (9) can be viewed as a Riemann-Stieltjes integral

$$\mathbf{u}^T f(A)\mathbf{v} = I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda). \tag{12}$$

As discussed in [6], the integral $I[f]$ can be approximated using Gaussian quadrature rules, which yield an approximation of the form

$$I[f] = \sum_{j=1}^{K} w_j f(t_j) + R[f], \tag{13}$$

where the nodes t_j, $j = 1, \ldots, K$, as well as the weights w_j, $j = 1, \ldots, K$, can be obtained using the symmetric Lanczos algorithm if $\mathbf{u} = \mathbf{v}$, and the unsymmetric Lanczos algorithm if $\mathbf{u} \neq \mathbf{v}$ (see [12]).

In the case $\mathbf{u} \neq \mathbf{v}$, there is the possibility that the weights may not be positive, which destabilizes the quadrature rule (see [13] for details). Instead, we consider

$$\begin{bmatrix} \mathbf{u} & \mathbf{v} \end{bmatrix}^T f(A) \begin{bmatrix} \mathbf{u} & \mathbf{v} \end{bmatrix}$$

which results in the 2×2 matrix

$$\int_a^b f(\lambda)\, d\mu(\lambda) = \begin{bmatrix} \mathbf{u}^T f(A)\mathbf{u} & \mathbf{u}^T f(A)\mathbf{v} \\ \mathbf{v}^T f(A)\mathbf{u} & \mathbf{v}^T f(A)\mathbf{v} \end{bmatrix}, \tag{14}$$

where $\mu(\lambda)$ is a 2×2 matrix function of λ, each entry of which is a measure of the form $\alpha(\lambda)$ from (11).

In [6] Golub and Meurant show how a block method can be used to generate quadrature formulas. We will describe this process here in more detail. The integral $\int_a^b f(\lambda)\, d\mu(\lambda)$ is now a 2×2 symmetric matrix and the most general K-node quadrature formula is of the form

$$\int_a^b f(\lambda)\, d\mu(\lambda) = \sum_{j=1}^{K} W_j f(T_j) W_j + error \tag{15}$$

with T_j and W_j being symmetric 2×2 matrices. By diagonalizing each T_j, we obtain the simpler formula

$$\int_a^b f(\lambda)\, d\mu(\lambda) = \sum_{j=1}^{2K} f(\lambda_j) \mathbf{v}_j \mathbf{v}_j^T + error, \tag{16}$$

where, for each j, λ_j is a scalar and $\mathbf{v}_j$ is a 2-vector.

Each node λ_j is an eigenvalue of the matrix

$$\mathscr{T}_K = \begin{bmatrix} M_1 & B_1^T & & & \\ B_1 & M_2 & B_2^T & & \\ & \ddots & \ddots & \ddots & \\ & & B_{K-2} & M_{K-1} & B_{K-1}^T \\ & & & B_{K-1} & M_K \end{bmatrix} \tag{17}$$

which is a symmetric block-triangular matrix of order $2K$. The vector $\mathbf{v}_j$ consists of the first two elements of the corresponding normalized eigenvector. To compute the matrices M_j and B_j, we use the block Lanczos algorithm, which was proposed by Golub and Underwood in [14].

We are now ready to describe block KSS methods. For each wave number $\omega = -N/2 + 1, \ldots, N/2$, we define

$$R_0(\omega) = \begin{bmatrix} \hat{\mathbf{e}}_\omega & \mathbf{u}^n \end{bmatrix}$$

and compute the QR factorization $R_0(\omega) = X_1(\omega) B_0(\omega)$. We then carry out block Lanczos iteration to obtain a block tridiagonal matrix $\mathscr{T}_K(\omega)$ of the form (17), where each entry is a function of ω.

Then, we can express each Fourier component of the approximate solution at the next time step as

$$[\hat{\mathbf{u}}^{n+1}]_\omega = \left[B_0^H E_{12}^H \exp[-\mathscr{T}_K(\omega)\Delta t] E_{12} B_0 \right]_{12} \tag{18}$$

where $E_{12} = \begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 \end{bmatrix}$. The computation of (18) consists of computing the eigenvalues and eigenvectors of $\mathscr{T}_K(\omega)$ in order to obtain the nodes and weights for Gaussian quadrature, as described earlier.

This algorithm has local temporal accuracy $O(\Delta t^{2K})$ [10]. Furthermore, block KSS methods are significantly more accurate than the original KSS methods described in [5, 8], even though they have the same temporal order of accuracy, because the solution plays a greater role in the determination of the quadrature nodes. They are also more effective for problems with oscillatory or discontinuous coefficients.

APPLICATION TO THE WAVE EQUATION

In this section we review the application of Krylov subspace spectral methods to the problem

$$u_{tt} + Lu = 0 \quad \text{on } (0,2\pi)\times(0,\infty), \tag{19}$$

$$u(x,0) = f(x), \quad u_t(x,0) = g(x), \quad 0 < x < 2\pi, \tag{20}$$

with periodic boundary conditions

$$u(0,t) = u(2\pi,t), \quad t > 0. \tag{21}$$

A spectral representation of the operator L allows us the obtain a representation of the solution operator (the *propagator*) in terms of the sine and cosine families generated by L by a simple functional calculus. Introduce

$$R_1(t) = L^{-1/2}\sin(t\sqrt{L}), \quad R_0(t) = \cos(t\sqrt{L}). \tag{22}$$

Then the propagator of (19) can be written as

$$P(t) = \begin{bmatrix} R_0(t) & R_1(t) \\ -LR_1(t) & R_0(t) \end{bmatrix}. \tag{23}$$

The entries of this matrix, as functions of L, indicate which functions are the integrands in the Riemann-Stieltjes integrals used to compute the Fourier components of the solution.

Block KSS methods can be applied to the wave equation in the same way as for parabolic problems, as described in the previous section, except that the block Lanczos algorithm is used twice for each Fourier coefficient, to compute the solution and its time derivative.

We now review the convergence analysis of block KSS methods carried out in [11].

Theorem 1 *Let L be a self-adjoint 2nd-order positive definite differential operator on $C_p([0,2\pi])$ with coefficients in $BL_M([0,2\pi])$ for a fixed integer M, and let $f,g \in C_p^n([0,2\pi])$ for $n \geq 4K$ for a positive integer K. Let $N \geq M$, and that for each $\omega = -N/2+1,\ldots,N/2$, the recursion coefficients in (17) are computed on a $2^K N$-point uniform grid. Then a block KSS method that uses a K-node block Gaussian rule to compute each Fourier component $[\hat{\mathbf{u}}^1]_\omega$, for $\omega = -N/2+1,\ldots,N/2$, of the solution to (19), (20), (21), and each Fourier component $[\hat{\mathbf{u}}_t^1]_\omega$ of its time derivative, satisfies*

$$\left|[\hat{\mathbf{u}}^1]_\omega - \hat{u}(\omega,\Delta t)\right| = O(\Delta t^{4K}), \quad \left|[\hat{\mathbf{u}}_t^1]_\omega - \hat{u}_t(\omega,\Delta t)\right| = O(\Delta t^{4K-1}),$$

where $\hat{u}(\omega,\Delta t)$ is the corresponding Fourier component of the exact solution at time Δt.

Proof. See [11, Theorem 5]. □

In [11, Theorem 6], it is shown that when the leading coefficient $p(x)$ is constant and the coefficient $q(x)$ is bandlimited, the 1-node KSS method, which has third-order local accuracy in time, is also unconditionally stable. This result, and Theorem 1, imply convergence for the 1-node method, with second-order global temporal accuracy.

APPLICATION TO MAXWELL'S EQUATIONS

In this section, we consider the various generalizations that must be made to block KSS methods for the wave equation in order to apply them to Maxwell's equations.

- First, we consider the following initial-boundary value problem in one space dimension,

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} + L\mathbf{u} = 0, \quad t > 0, \tag{24}$$

  with periodic boundary conditions, where $\mathbf{u} : [0,2\pi]\times[0,\infty) \to \mathbb{R}^n$ for $n > 1$, and $L(x,D)$ is an $n\times n$ matrix where the (i,j) entry is an a differential operator $L_{ij}(x,D)$ of the form

$$L_{ij}(x,D)u(x) = \sum_{\mu=0}^{m_{ij}} a_\mu^{ij}(x)D^\mu u, \quad D = \frac{d}{dx}, \tag{25}$$

with spatially varying coefficients a_μ^{ij}, $\mu = 0, 1, \ldots, m_{ij}$.

Generalization of KSS methods to a system of the form (24) can proceed as follows. For $i, j = 1, \ldots, n$, let $\overline{L}_{ij}(D)$ be the constant-coefficient operator obtained by averaging the coefficients of $L_{ij}(x, D)$ over $[0, 2\pi]$. Then, for each wave number ω, we define $L(\omega)$ be the matrix with entries $\overline{L}_{ij}(\omega)$, i.e., the symbols of $\overline{L}_{ij}(D)$ evaluated at ω. Next, we compute the spectral decomposition of $L(\omega)$ for each ω. For $j = 1, \ldots, n$, let $\mathbf{q}_j(\omega)$ be the left eigenvectors of $L(\omega)$. Then, we define our test functions by $\mathbf{q}_j(\omega) \otimes e^{i\omega x}$, and the trial functions are defined similarly using the right eigenvectors.

The recursion coefficients, nodes and weights can be computed in the same manner as in the scalar, self-adjoint case, with obvious modifications to account for the fact that the matrix $T_\omega(\delta_\omega)$, for each ω, is no longer Hermitian. Once the components of the solution in our basis of trial functions is computed, the Fourier coefficients of each component function can be computed by solving nN linear systems of size $n \times n$.

- As shown in [15, 11], rough or discontinuous coefficients reduce the accuracy of KSS methods, because they introduce significant spatial discretization error into the computation of recursion coefficients.

  Alternatively, adaptive spatial resolution has been shown to be effective for handling multilayer profiles in TE and TM polarizations (see [16]), which KSS methods can readily incorporate as well. Ongoing work also explores the use of reprojection techniques (see, for example, [17]).
- While we have used periodic boundary conditions in this paper, it is typical in practical applications to use boundary conditions that are more effective at simulating an infinite domain. One such type of boundary condition is a perfectly matched layer (PML), first used by Berenger in [18] for Maxwell's equations. A PML absorbs waves by modifying spatial differentiation operators in the PDE. For example, for absorbing waves that propagate in the x direction, $\frac{\partial}{\partial x}$ is replaced by $\frac{1}{1+\frac{i\sigma(x)}{\omega}}\frac{\partial}{\partial x}$, where, as before, ω represents the wave number, and σ is a positive function that causes propagating waves to be attenuated.

  In KSS methods, this transformation can be incorporated into the symbol of the operator L when computing the recursion coefficients. The dependence of the transformation on both x and ω makes the efficient application of the transformed operator more difficult, especially in higher space dimensions, but recent work on rapid application of Fourier integral operators (see [19]) can mitigate this concern.

NUMERICAL RESULTS

We now apply a 2-node block KSS method to the equation (2), with initial conditions

$$\hat{\mathbf{E}}(x, y, z, 0) = \mathbf{F}(x, y, z), \quad \frac{\partial \hat{\mathbf{E}}}{\partial t}(x, y, z, 0) = \mathbf{G}(x, y, z), \tag{26}$$

with periodic boundary conditions. The coefficients μ and ε are constructed from randomly generated, damped Fourier coefficients as described in [5]. The components of $\mathbf{F}$ and $\mathbf{G}$ are generated in a similar fashion, except that the x- and z-components are zero. Table 1 lists error estimates for solutions computed using $K = 2$ block quadrature nodes per component in the basis described in the previous section. We observe that as the number of grid points increases, the temporal order of accuracy also increases toward the theoretical expectation of 6th-order accuracy, due to the reduced spatial error arising from the truncation of Fourier series. Also, increasing the resolution does not pose any difficulty from a stability point of view; for a fixed time step, accuracy increases with resolution.

CONCLUSIONS

We have demonstrated that KSS methods can be applied to Maxwell's equations with smoothly varying coefficients. The temporal accuracy is the same as for the wave equation, even though Fourier components are now represented by bilinear forms involving non-self-adjoint matrices, which are treated as Riemann-Stieltjes integrals over contours in the complex plane. Future work will extend the approach described in this paper to more realistic applications by using symbol modification to efficiently implement perfectly matched layers, and various techniques to effectively handle discontinuous coefficients.

TABLE 1. Estimates of relative error in solutions of (2), (26) computed using a 2-node block KSS method on an N-point grid, with time step Δt, for various values of N and Δt. For each N, the order of convergence is measured using the error estimates from time steps 1 and $1/32$.

Δt	$N = 16$, Order=5.52	$N = 32$, Order=5.84
1	6.654e-3	3.641e-3
1/2	2.577e-4	7.466e-5
1/4	3.233e-6	8.301e-7
1/8	4.888e-8	9.432e-9
1/16	7.656e-10	1.571e-10
1/32	3.264e-11	5.922e-12

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