A Spectral Time-Domain Method for Computational Electrodynamics

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Abstract Block Krylov subspace spectral (KSS) methods have previously been applied to the variable-coefficient heat equation and wave equation, and have demonstrated high-order accuracy, as well as stability characteristic of implicit time-stepping schemes, even though KSS methods are explicit. 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 non-self-adjoint systems of coupled equations, such as Maxwell's equations.

1 Introduction

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

$$\operatorname{div}\hat{\mathbf{E}} = 0, \quad \operatorname{div}\hat{\mathbf{H}} = 0, \tag{1}$$

$$\operatorname{curl}\hat{\mathbf{E}} = -\mu\frac{\partial\hat{\mathbf{H}}}{\partial t}, \quad \operatorname{curl}\hat{\mathbf{H}} = \varepsilon\frac{\partial\hat{\mathbf{E}}}{\partial t}, \tag{2}$$

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.

By taking the curl of both sides of (2), we decouple the vector fields $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$ and obtain the equations

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$$\mu\varepsilon\frac{\partial^2\hat{\mathbf{E}}}{\partial t^2} = \Delta\hat{\mathbf{E}} + \mu^{-1}\text{curl}\,\hat{\mathbf{E}}\times\nabla\mu, \tag{3}$$

$$\mu\varepsilon\frac{\partial^2\hat{\mathbf{H}}}{\partial t^2} = \Delta\hat{\mathbf{H}} + \varepsilon^{-1}\text{curl}\,\hat{\mathbf{H}}\times\nabla\varepsilon. \tag{4}$$

In his 1966 paper [17], Yee proposed the original finite-difference time-domain method for solving the equations (1), (2). 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. In this paper, we introduce a new time-domain method for these equations.

In [14] 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 [4] for approximating elements of a function of a matrix by Gaussian quadrature in the *spectral* domain. In [8, 10], these methods were generalized to the second-order 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 coefficient 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 [10], they are also quite stable, considering that they are explicit methods. In [11, 12], the accuracy and robustness of KSS methods were enhanced using block Gaussian quadrature.

Our goal is to extend the high-order accuracy achieved for the scalar wave equation to systems of coupled wave equations such as those described by Maxwell's equations. Section 2 reviews the main properties of KSS methods, including block KSS methods, as applied to the parabolic problems for which they were originally designed. Section 3 reviews their application to the wave equation, including previous convergence analysis. In Section 4, we discuss the modifications that must be made to block KSS methods in order to apply them to Maxwell's equations. Numerical results are presented in Section 5, and conclusions are stated in Section 6.

2 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

$$u_t + Lu = 0, \quad t > 0, \tag{5}$$

with appropriate initial conditions and periodic boundary conditions. The operator L is a second-order, self-adjoint, positive definite differential operator.

Let $\langle\cdot,\cdot\rangle$ denote the standard inner product of functions defined on $[0, 2\pi]$. Krylov subspace spectral methods, introduced in [14], use Gaussian quadrature on the spectral domain to compute the Fourier coefficients 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 coefficients that would be obtained by applying the exact solution operator to $\tilde{u}(x,t_n)$,

$$\hat{u}(\omega,t_{n+1}) = \left\langle \frac{1}{\sqrt{2\pi}} e^{i\omega x}, S(\Delta t)\tilde{u}(x,t_n) \right\rangle. \tag{6}$$

In [4] Golub and Meurant describe a method for computing quantities of the form

$$\mathbf{u}^T f(A)\mathbf{v}, \tag{7}$$

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 obtained 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

$$b = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N = a > 0, \tag{8}$$

and corresponding orthogonal eigenvectors $\mathbf{q}_j$, $j = 1, \ldots, N$. Therefore, the quantity (7) can be rewritten as

$$\mathbf{u}^T f(A)\mathbf{v} = \sum_{j=1}^{N} f(\lambda_j)\mathbf{u}^T \mathbf{q}_j \mathbf{q}_j^T \mathbf{v}. \tag{9}$$

which can also be viewed as a Riemann-Stieltjes integral

$$\mathbf{u}^T f(A)\mathbf{v} = I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda). \tag{10}$$

As discussed in [4], the integral $I[f]$ can be approximated using Gaussian quadrature rules, which yields an approximation of the form

$$I[f] = \sum_{j=1}^{K} w_j f(\lambda_j) + R[f], \tag{11}$$

where the nodes λ_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 [7]).

In the case $\mathbf{u} \neq \mathbf{v}$, there is a possibility that the weights may not be positive, which destabilizes the quadrature rule (see [1] for details). Instead, we consider

$$\left[\mathbf{u}\ \mathbf{v}\right]^T f(A) \left[\mathbf{u}\ \mathbf{v}\right], \tag{12}$$

which results in the 2×2 matrix

$$\int_a^b f(\lambda)\,d\mu(\lambda) = \begin{bmatrix} \mathbf{u}^T f(A)\mathbf{u} & \mathbf{u}^T f(A)\mathbf{v} \\ \mathbf{v}^T f(A)\mathbf{u} & \mathbf{v}^T f(A)\mathbf{v} \end{bmatrix}, \tag{13}$$

where $\mu(\lambda)$ is a 2×2 matrix function of λ, each entry of which is a measure of the form $\alpha(\lambda)$ from (10).

In [4] Golub and Meurant showed 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

$$\int_a^b f(\lambda)\,d\mu(\lambda) = \sum_{j=1}^{K} W_j f(T_j) W_j + error, \tag{14}$$

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

$$\int_a^b f(\lambda)\,d\mu(\lambda) = \sum_{j=1}^{2K} f(\lambda_j)\mathbf{v}_j\mathbf{v}_j^T + error, \tag{15}$$

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

$$\mathscr{T}_K = \begin{bmatrix} M_1 & B_1^T & & & \\ B_1 & M_2 & B_2^T & & \\ & \ddots & \ddots & \ddots & \\ & & B_{K-2} & M_{K-1} & B_{K-1}^T \\ & & & B_{K-1} & M_K \end{bmatrix}, \tag{16}$$

which is a 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 [6].

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

$$R_0(\omega) = \left[\hat{\mathbf{e}}_\omega\ \mathbf{u}^n\right]$$

and compute the QR factorization $R_0(\omega) = X_1(\omega)B_0(\omega)$. We then carry out block Lanczos iteration, applied to the discretized operator L_N, to obtain a block tridiagonal matrix $\mathscr{T}_K(\omega)$ of the form (16), where each entry is a function of ω. The recursion coefficents in $\mathscr{T}_K(\omega)$ can be computed efficiently by applying basic rules of symbolic calculus, including in higher spatial dimensions.

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

$$[\hat{\mathbf{u}}^{n+1}]_\omega = \left[B_0^H E_{12}^H \exp[-\mathscr{T}_K(\omega)\Delta t] E_{12} B_0\right]_{12} \tag{17}$$

where $E_{12} = \left[\mathbf{e}_1\ \mathbf{e}_2\right]$. The computation of (17) 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 $O(\Delta t^{2K-1})$ [11]. Furthermore, block KSS methods are more accurate than the original KSS methods described in [10, 14], even though they have the same order of accuracy, because the solution $\mathbf{u}^n$ plays a greater role in the determination of the quadrature nodes. They are also more effective for problems with oscillatory or discontinuous coefficients [11].

3 Application to the Wave Equation

In this section, we review the application of Krylov subspace spectral methods to the wave equation

$$u_{tt} + Lu = 0 \quad \text{on } (0,2\pi)\times(0,\infty), \tag{18}$$

with appropriate initial conditions, and periodic boundary conditions. A spectral representation of the operator L allows us to 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

$$R_1(t) = L^{-1/2}\sin(t\sqrt{L}) = \sum_{n=1}^{\infty} \frac{\sin(t\sqrt{\lambda_n})}{\sqrt{\lambda_n}} \langle \varphi_n^*, \cdot \rangle \varphi_n, \tag{19}$$

$$R_0(t) = \cos(t\sqrt{L}) = \sum_{n=1}^{\infty} \cos(t\sqrt{\lambda_n}) \langle \varphi_n^*, \cdot \rangle \varphi_n, \tag{20}$$

where $\lambda_1, \lambda_2, \ldots$ are the (positive) eigenvalues of L, and $\varphi_1, \varphi_2, \ldots$ are the corresponding eigenfunctions. Then the propagator of (18) can be written as

$$P(t) = \begin{bmatrix} R_0(t) & R_1(t) \\ -LR_1(t) & R_0(t) \end{bmatrix}. \tag{21}$$

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 coefficients of the solution.

In [12, 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 second-order local accuracy in time, is also unconditionally stable. In general, as shown in [12], the local temporal error is $O(\Delta t^{4K-2})$ when K block Gaussian nodes are used for each Fourier coefficient.

4 Application to Maxwell's Equations

In this section, we consider generalizations that must be made to block KSS methods for the wave equation in order to apply them to a non-self-adjoint system of coupled equations such as (3).

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

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} + L\mathbf{u} = 0, \quad t > 0, \tag{22}$$

with appropriate initial conditions, and 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

$$L_{ij}(x,D)u(x) = \sum_{\mu=0}^{m_{ij}} a_\mu^{ij}(x) D^\mu u, \quad D = \frac{d}{dx}, \tag{23}$$

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

Generalization of KSS methods to a system of the form (22) 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 Schur vectors of $L(\omega)$. Then, we define our test and trial functions by $\phi_{j,\omega}(x) = \mathbf{q}_j(\omega) \otimes e^{i\omega x}$.

For Maxwell's equations, the matrix A_N that discretizes the operator

$$A\hat{\mathbf{E}} = \frac{1}{\mu\varepsilon}\left(\Delta\hat{\mathbf{E}} + \mu^{-1}\mathrm{curl}\,\hat{\mathbf{E}} \times \nabla\mu\right)$$

is not symmetric, and for each coefficient of the solution, the resulting quadrature nodes λ_j, $j = 1,\ldots,2K$, from (15) are now complex and must be obtained by a straightforward modification of block Lanczos iteration for unsymmetric matrices.

5 Numerical Results

We now apply a 2-node block KSS method to the equation (3), with initial conditions

$$\hat{\mathbf{E}}(x,y,z,0) = \mathbf{F}(x,y,z), \quad \frac{\partial\hat{\mathbf{E}}}{\partial t}(x,y,z,0) = \mathbf{G}(x,y,z), \tag{24}$$

with periodic boundary conditions. The coefficients μ and ε are given by

$$\mu(x,y,z) = 0.4077 + 0.0039\cos z + 0.0043\cos y - 0.0012\sin y +$$

$$0.0018\cos(y+z)+0.0027\cos(y-z)+0.003\cos x+$$
$$0.0013\cos(x-z)+0.0012\sin(x-z)+0.0017\cos(x+y)+$$
$$0.0014\cos(x-y), \tag{25}$$

$$\varepsilon(x,y,z) = 0.4065+0.0025\cos z+0.0042\cos y+0.001\cos(y+z)+$$
$$0.0017\cos x+0.0011\cos(x-z)+0.0018\cos(x+y)+$$
$$0.002\cos(x-y). \tag{26}$$

The components of **F** and **G** are generated in a similar fashion, except that the x- and z-components are zero.

Figure 1 demonstrates the convergence behavior using error estimates for solutions computed using $K=2$ block quadrature nodes per coefficient in the basis described in Section 4. Since the exact solution is not available, the error estimate for each solution is obtained by taking the ℓ_2-norm of the relative difference between the y-component of the solution, and that of a solution computed using a smaller time step $\Delta t = 1/64$ and the maximum number of grid points.

At both spatial resolutions, the scheme exhibits approximately 6th-order accuracy in time as Δt decreases, except that for $N=16$, the spatial error arising from truncation of Fourier series is significant enough that the overall error fails to decrease below the level achieved at $\Delta t = 1/8$. For $N=32$, the solution is sufficiently resolved in space, and the order of overgence as $\Delta t \to 0$ is approximately 6.1.

We also note that increasing the resolution does not pose any difficulty from a stability point of view. Unlike explicit finite-difference schemes that are constrained by a CFL condition, KSS methods do not require a reduction in the time step to offset a reduction in the spatial step in order to maintain boundedness of the solution, because their domain of dependence includes the entire spatial domain for any Δt.

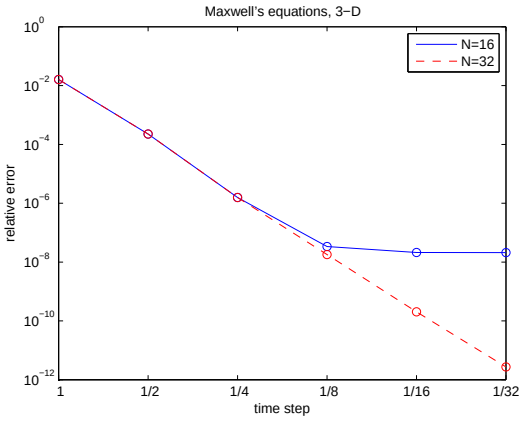

Fig. 1 Estimates of relative error in solutions of (3), (24) computed using a 2-node block KSS method on an N-point grid, with time step Δt, for various values of N and Δt.

6 Conclusions

We have demonstrated that KSS methods can be applied to Maxwell's equations with smoothly varying coefficients. The order of temporal accuracy is the same as for the wave equation, even though Fourier coefficients 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 (see [2]), and various techniques (see [3, 16]) to effectively handle discontinuous coefficients.

References

1. Atkinson, K.: *An Introduction to Numerical Analysis, 2nd Ed.* Wiley (1989)
2. Berenger, J,: A perfectly matched layer for the absorption of electromagnetic waves. *J. Comp. Phys.* **114** (1994) 185-200.
3. Gelb, A., Tanner, J.: Robust Reprojection Methods for the Resolution of the Gibbs Phenomenon. *Appl. Comput. Harmon. Anal.* **20** (2006) 3-25.
4. Golub, G. H., Meurant, G.: Matrices, Moments and Quadrature. *Proceedings of the 15th Dundee Conference*, June-July 1993, Griffiths, D. F., Watson, G. A. (eds.), Longman Scientific & Technical (1994)
5. Golub, G. H., Gutknecht, M. H.: Modified Moments for Indefinite Weight Functions. *Numerische Mathematik* **57** (1989) 607-624.
6. Golub, G. H., Underwood, R.: The block Lanczos method for computing eigenvalues. *Mathematical Software III*, J. Rice Ed., (1977) 361-377.
7. Golub, G. H, Welsch, J.: Calculation of Gauss Quadrature Rules. *Math. Comp.* **23** (1969) 221-230.
8. Guidotti, P., Lambers, J. V., Sølna, K.: Analysis of 1-D Wave Propagation in Inhomogeneous Media. *Numerical Functional Analysis and Optimization* **27** (2006) 25-55.
9. Hochbruck, M., Lubich, C.: On Krylov Subspace Approximations to the Matrix Exponential Operator. *SIAM Journal of Numerical Analysis* **34** (1996) 1911-1925.
10. Lambers, J. V.: Derivation of High-Order Spectral Methods for Time-dependent PDE using Modified Moments. *Electronic Transactions on Numerical Analysis* **28** (2008) 114-135.
11. Lambers, J. V.: Enhancement of Krylov Subspace Spectral Methods by Block Lanczos Iteration. *Electronic Transactions on Numerical Analysis* **31** (2008) 86-109.
12. Lambers, J. V.: An Explicit, Stable, High-Order Spectral Method for the Wave Equation Based on Block Gaussian Quadrature. *IAENG Journal of Applied Mathematics* **38** (2008) 333-348.
13. Lambers, J. V.: Krylov Subspace Spectral Methods for the Time-Dependent Schrödinger Equation with Non-Smooth Potentials. *Numerical Algorithms* **51** (2009) 239-280.
14. Lambers, J. V.: Krylov Subspace Spectral Methods for Variable-Coefficient Initial-Boundary Value Problems. *Electronic Transactions on Numerical Analysis* **20** (2005) 212-234.
15. Lambers, J. V.: Practical Implementation of Krylov Subspace Spectral Methods. *Journal of Scientific Computing* **32** (2007) 449-476.
16. Vallius, T., Honkanen, M.: Reformulation of the Fourier nodal method with adaptive spatial resolution: application to multilevel profiles. *Opt. Expr.* **10**(1) (2002) 24-34.
17. Yee, K.: Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media. *Ant. Prop., IEEE Trans.* **14** (1966) 302-307.