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Spectral Methods for Time-dependent Variable-coefficient PDE Based on Block Gaussian Quadrature

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Abstract—**Block Krylov subspace spectral (KSS) methods are a "best-of-both-worlds" compromise between explicit and implicit time-stepping methods for variable-coefficient PDE, in that they combine the efficiency of explicit methods and the stability of implicit methods, while also achieving spectral accuracy in space and high-order accuracy in time. Block KSS methods compute each Fourier coefficient of the solution using techniques developed by Gene Golub and Gérard Meurant for approximating elements of functions of matrices by block Gaussian quadrature in the spectral, rather than physical, domain. This paper describes how block KSS methods can be applied to a variety of equations, and also demonstrates their superiority, in terms of accuracy and efficiency, to other Krylov subspace methods in the literature.**

Keywords: spectral methods, Gaussian quadrature, block Lanczos method, Maxwell's equation, heat equation

1 Introduction

In [11] a class of methods, called block 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 [12], 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 they are also quite stable, considering that they are explicit methods. They are also effective for solving systems of coupled equations, such as Maxwell's equations [16].

In this paper, we review block KSS methods, as applied to various types of PDE, and compare their performance to other Krylov subspace methods from the literature. Section 2 reviews the main properties of block KSS methods, as applied to the parabolic problems for which they were designed. Section 3 discusses implementation details, and demonstrates why KSS methods need to explicitly generate only one Krylov subspace, although information from several is used. In Section 4, we discuss modifications that must be made to block KSS methods in order to apply them to systems of coupled wave equations, such as 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 block KSS methods, which are easier to describe for parabolic problems. Let $S(t) = \exp[-Lt]$ represent the exact solution operator of the problem

$$u_t + Lu = 0, \quad t > 0, \tag{1}$$

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 $[0, 2\pi]$. Block Krylov subspace spectral methods, introduced in [11], 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 $\tilde{u}(x, t_n)$,

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

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

$$\mathbf{u}^T f(A)\mathbf{v}, \tag{3}$$

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

$$b = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N = a > 0, \tag{4}$$

and corresponding orthogonal eigenvectors $\mathbf{q}_j$, $j = 1, \ldots, N$. Therefore, the quantity (3) can be rewritten as

$$\mathbf{u}^T f(A)\mathbf{v} = \sum_{j=1}^{N} f(\lambda_j)\mathbf{u}^T \mathbf{q}_j \mathbf{q}_j^T \mathbf{v}. \tag{5}$$

which can also be viewed as a Riemann-Stieltjes integral

$$\mathbf{u}^T f(A)\mathbf{v} = I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda). \tag{6}$$

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

$$I[f] = \sum_{j=1}^{K} w_j f(\lambda_j) + R[f], \tag{7}$$

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

$$\begin{bmatrix} \mathbf{u} & \mathbf{v} \end{bmatrix}^T f(A) \begin{bmatrix} \mathbf{u} & \mathbf{v} \end{bmatrix}, \tag{8}$$

which results in the 2×2 matrix

$$\int_a^b f(\lambda)\, d\mu(\lambda) = \begin{bmatrix} \mathbf{u}^T f(A)\mathbf{u} & \mathbf{u}^T f(A)\mathbf{v} \\ \mathbf{v}^T f(A)\mathbf{u} & \mathbf{v}^T f(A)\mathbf{v} \end{bmatrix}, \tag{9}$$

where $\mu(\lambda)$ is a 2×2 matrix function of λ, each entry of which is a measure of the form $\alpha(\lambda)$ from (6).

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

$$\int_a^b f(\lambda)\, d\mu(\lambda) = \sum_{j=1}^{K} W_j f(T_j) W_j + error, \tag{10}$$

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

$$\int_a^b f(\lambda)\, d\mu(\lambda) = \sum_{j=1}^{2K} f(\lambda_j)\mathbf{v}_j \mathbf{v}_j^T + error, \tag{11}$$

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

$$\mathcal{T}_K = \begin{bmatrix} M_1 & B_1^T & & & \\ B_1 & M_2 & B_2^T & & \\ & \ddots & \ddots & \ddots & \\ & & B_{K-2} & M_{K-1} & B_{K-1}^T \\ & & & B_{K-1} & M_K \end{bmatrix}, \tag{12}$$

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 $R_0(\omega) = \begin{bmatrix} \hat{\mathbf{e}}_\omega & \mathbf{u}^n \end{bmatrix}$ and compute the QR factorization $R_0(\omega) = X_1(\omega)B_0(\omega)$. We then carry out block Lanczos iteration, applied to the discretized operator L_N, to obtain a block tridiagonal matrix $\mathcal{T}_K(\omega)$ of the form (12), where each entry is a function of ω.

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

$$[\hat{\mathbf{u}}^{n+1}]_\omega = \left[B_0^H E_{12}^H \exp[-\mathcal{T}_K(\omega)\Delta t] E_{12} B_0\right]_{12} \tag{13}$$

where $E_{12} = \begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 \end{bmatrix}$. The computation of (13) consists of computing the eigenvalues and eigenvectors of $\mathcal{T}_K(\omega)$ 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 [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

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for problems with oscillatory or discontinuous coefficients [11].

Block KSS methods are even more accurate for the second-order wave equation, for which block Lanczos iteration is used to compute both the solution and its time derivative. In [12, Theorem 6], it is shown that when the leading coefficient is constant and the coefficient $q(x)$ is bandlimited, the 1-node KSS method, which has second-order 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.

3 Implementation

KSS methods compute a Jacobi matrix corresponding to *each* Fourier coefficient, in contrast to traditional Krylov subspace methods that normally use only a single Krylov subspace generated by the initial data or the solution from the previous time step. While it would appear that KSS methods incur a substantial amount of additional computational expense, that is not actually the case, because nearly all of the Krylov subspaces that they compute are closely related by the wave number ω, in the 1-D case, or $\vec{\omega} = (\omega_1, \omega_2, \ldots, \omega_n)$ in the n-D case.

In fact, the only Krylov subspace that is explicitly computed is the one generated by the solution from the previous time step, of dimension $(K+1)$, where K is the number of block Gaussian quadrature nodes. In addition, the averages of the coefficients of L^j, for $j = 0, 1, 2, \ldots, 2K-1$, are required, where L is the spatial differential operator. When the coefficients of L are independent of time, these can be computed once, during a preprocessing step. This computation can be carried out in $O(N \log N)$ operations using symbolic calculus [13, 15].

With these considerations, the algorithm for a single time step of a 1-node block KSS method for solving (1), where $Lu = -pu_{xx} + q(x)u$, with appropriate initial conditions and periodic boundary conditions, is as follows. We denote the average of a function $f(x)$ on $[0, 2\pi]$ by $\overline{f}$, and the computed solution at time t_n by u^n.

$\hat{u}^n = \mathbf{fft}(u^n)$, $v = Lu^n$, $\hat{v} = \mathbf{fft}(v)$
for each ω **do**
  $\alpha_1 = -p\omega^2 + \overline{q}$ (in preprocessing step)
  $\beta_1 = \hat{v}(\omega) - \alpha_1 \hat{u}^n(\omega)$
  $\alpha_2 = \langle u^n, v\rangle - 2\,\mathrm{Re}\,[\hat{u}^n(\omega)\overline{v(\omega)}] + \alpha_1 |u^n(\omega)|^2$
  $e_\omega = [\langle u^n, u^n\rangle - |\hat{u}^n(\omega)|^2]^{1/2}$
  $T_\omega = \begin{bmatrix} \alpha_1 & \beta_1/e_\omega \\ \beta_1/e_\omega & \alpha_2/e_\omega^2 \end{bmatrix}$
  $\hat{u}^{n+1}(\omega) = [e^{-T_\omega \Delta t}]_{11} \hat{u}^n(\omega) + [e^{-T_\omega \Delta t}]_{12} e_\omega$
end
$u^{n+1} = \mathbf{ifft}(\hat{u}^{n+1})$

It should be noted that for a parabolic problem such as (1), the loop over ω only needs to account for non-negligible Fourier coefficients of the solution, which are relatively few due to the smoothness of solutions to such problems.

4 Application to Maxwell's Equations

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

$$\mathrm{div}\,\hat{\mathbf{E}} = 0, \quad \mathrm{div}\,\hat{\mathbf{H}} = 0, \tag{14}$$

$$\mathrm{curl}\,\hat{\mathbf{E}} = -\mu \frac{\partial \hat{\mathbf{H}}}{\partial t}, \quad \mathrm{curl}\,\hat{\mathbf{H}} = \varepsilon \frac{\partial \hat{\mathbf{E}}}{\partial t}, \tag{15}$$

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.

Taking the curl of both sides of (15) yields

$$\mu\varepsilon \frac{\partial^2 \hat{\mathbf{E}}}{\partial t^2} = \Delta \hat{\mathbf{E}} + \mu^{-1} \mathrm{curl}\,\hat{\mathbf{E}} \times \nabla \mu, \tag{16}$$

$$\mu\varepsilon \frac{\partial^2 \hat{\mathbf{H}}}{\partial t^2} = \Delta \hat{\mathbf{H}} + \varepsilon^{-1} \mathrm{curl}\,\hat{\mathbf{H}} \times \nabla \varepsilon. \tag{17}$$

In this section, we discuss generalizations that must be made to block KSS methods in order to apply them to a non-self-adjoint system of coupled equations such as (16). Additional details are given in [16].

First, we consider the following 1-D problem,

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} + L\mathbf{u} = 0, \quad t > 0, \tag{18}$$

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

$$L_{ij}(x, D)u(x) = \sum_{\mu=0}^{m_{ij}} a_\mu^{ij}(x) D^\mu u, \quad D = \frac{d}{dx}, \tag{19}$$

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

Generalization of KSS methods to a system of the form (18) 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.

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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 $\vec{\phi}_{j,\omega}(x) = \mathbf{q}_j(\omega) \otimes e^{i\omega x}$.

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

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

is not symmetric, and for each coefficient of the solution, the resulting quadrature nodes λ_j, $j = 1, \ldots, 2K$, from (11) are now complex and must be obtained by a straightforward modification of block Lanczos iteration for unsymmetric matrices.

5 Numerical Results

In this section, we compare the performance of block KSS methods with various methods based on exponential integrators [8, 10, 19].

5.1 Parabolic Problems

We first consider a 1-D parabolic problem of the form (1), where the differential operator L is defined by $Lu(x) = -pu''(x) + q(x)u(x)$, where $p \approx 0.4$ and

$$\begin{aligned} q(x) \quad \approx \quad & -0.44 + 0.03\cos x - 0.02\sin x + 0.005\cos 2x - \\ & 0.004\sin 2x + 0.0005\cos 3x \end{aligned}$$

is constructed so as to have the smoothness of a function with three continuous derivatives, as is the initial data $u(x, 0)$. Periodic boundary conditions are imposed.

We solve this problem using the following methods:

- A 2-node block KSS method. Each time step requires construction of a Krylov subspace of dimension 3 generated by the solution, and the coefficients of L^2 and L^3 are computed during a preprocessing step.
- A preconditioned Lanczos iteration for approximating $e^{-\tau A}\mathbf{v}$, introduced in [17] for approximating the matrix exponential of sectorial operators, and adapted in [19] for efficient application to the solution of parabolic PDE. In this approach, Lanczos iteration is applied to $(I+hA)^{-1}$, where h is a parameter, in order to obtain a restricted rational approximation of the matrix exponential. We use $m = 4$ and $m = 8$ Lanczos iterations, and choose $h = \Delta t/10$, as in [19].
- A method based on exponential integrators, from [8], that is of order 3 when the Jacobian is approximated to within $O(\Delta t)$. We use $m = 8$ Lanczos iterations.

Since the exact solution is not available, the error is estimated by taking the ℓ_2-norm of the relative difference between each solution, and that of a solution computed using a smaller time step $\Delta t = 1/64$ and the maximum number of grid points.

The results are shown in Figures 1 and 2. As the number of grid points is doubled, only the block KSS method shows an improvement in accuracy; the preconditioned Lanczos method exhibits a slight degradation in performance, while the explicit fourth-order exponential integrator-based method requires that the time step be reduced by a factor of 4 before it can deliver the expected order of convergence; similar behavior was demonstrated for an explicit 3rd-order method from [9] in [14].

The preconditioned Lanczos method requires 8 Lanczos iterations to match the accuracy of a block KSS method that uses only 2. On the other hand, the block KSS method incurs additional expense due to (1) the computation of the moments of L, for each Fourier coefficient, and (2) the exponentiation of separate Jacobi matrices for each Fourier coefficient. These expenses are mitigated by the fact that the first takes place once, during a preprocessing stage, and both tasks require an amount of work that is proportional not to the number of grid points, but to the number of non-negligible Fourier coefficients of the solution.

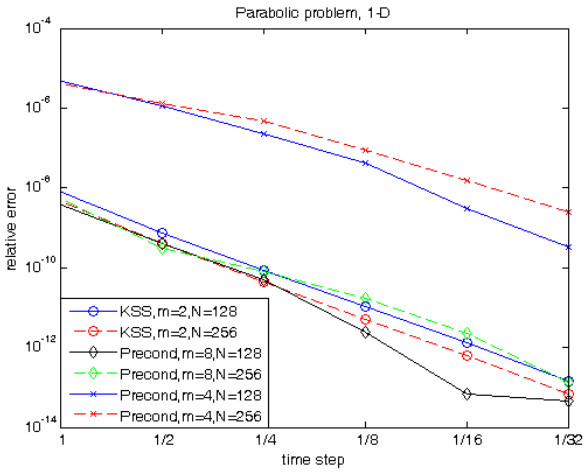

Figure 1: Estimates of relative error at $t = 0.1$ in solutions of (1) computed using preconditioned exponential integrator [19] with 4 and 8 Lanczos iterations, and a 2-node block KSS method. All methods compute solutions on an N-point grid, with time step Δt, for various values of N and Δt.

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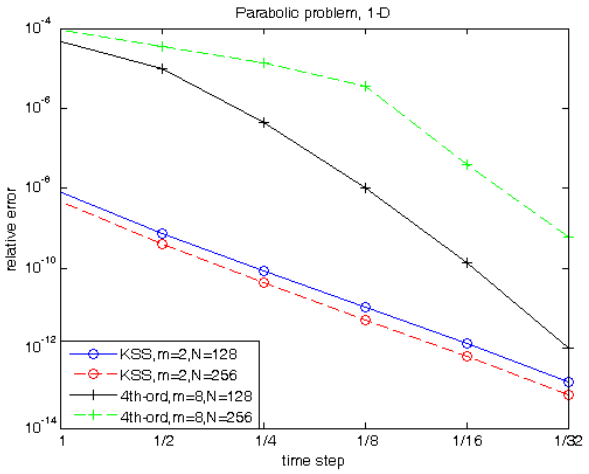

Figure 2: Estimates of relative error at $t = 0.1$ in solutions of (1) computed using a 4th-order method based on an exponential integrator [10] with 8 Lanczos iterations, and a 2-node block KSS method. Both methods compute solutions on an N-point grid, with time step Δt, for various values of N and Δt.

5.2 Maxwell's Equations

We now apply a 2-node block KSS method to (16), with initial conditions

$$\hat{\mathbf{E}}(x,y,z,0) = \mathbf{F}(x,y,z), \quad \frac{\partial \hat{\mathbf{E}}}{\partial t}(x,y,z,0) = \mathbf{G}(x,y,z), \tag{20}$$

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

$$\begin{aligned}
\mu(x,y,z) &= 0.4077 + 0.0039\cos z + 0.0043\cos y - \\
&\quad 0.0012\sin y + 0.0018\cos(y+z) + \\
&\quad 0.0027\cos(y-z) + 0.003\cos x + \\
&\quad 0.0013\cos(x-z) + 0.0012\sin(x-z) + \\
&\quad 0.0017\cos(x+y) + 0.0014\cos(x-y), \\
\varepsilon(x,y,z) &= 0.4065 + 0.0025\cos z + 0.0042\cos y + \\
&\quad 0.001\cos(y+z) + 0.0017\cos x + \\
&\quad 0.0011\cos(x-z) + 0.0018\cos(x+y) + \\
&\quad 0.002\cos(x-y).
\end{aligned}$$

The components of $\mathbf{F}$ and $\mathbf{G}$ are generated in a similar fashion, except that the x- and z-components are zero.

We use a block KSS method that uses $K = 2$ block quadrature nodes per coefficient in the basis described in Section 4, that is 6th-order accurate in time, and a cosine method based on a Gautschi-type exponential integrator [8, 10]. This method is second-order in time, and in these experiments, we use $m = 2$ Lanczos iterations to approximate the Jacobian. It should be noted that when m is increased, even to a substantial degree, the results are negligibly affected.

Figure 3 demonstrates the convergence behavior for both methods. At both spatial resolutions, the block KSS method 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.

The Gautschi-type exponential integrator method is second-order accurate, as expected, and delivers nearly identical results for both spatial resolutions, but even with a Krylov subspace of much higher dimension than that used in the block KSS method, it is only able to achieve at most second-order accuracy, whereas a block KSS method, using a Krylov subsapce of dimension 3, achieves sixth-order accuracy. This is due to the incorporation of the moments of the spatial differential operator into the computation, and the use of Gaussian quadrature rules specifically tailored to each Fourier coefficient.

6 Summary and Future Work

We have demonstrated that block KSS methods can be applied to Maxwell's equations with smoothly varying coefficients, by appropriate generalization of their application to the scalar second-order wave equation, in a way that preserves the order of accuracy achieved for the wave equation. Furthermore, it has been demonstrated that while traditional Krylov subspace methods based on exponential integrators are most effective for parabolic problems, especially when aided by preconditioning as in [19], KSS methods perform best when applied to hyperbolic problems, in view of their much higher order of accuracy. Future work will extend the approach described in this paper to more realistic applications involving Maxwell's equations by using symbol modification to efficiently implement perfectly matched layers (see [2]), and various techniques (see [3, 18]) to effectively handle discontinuous coefficients.

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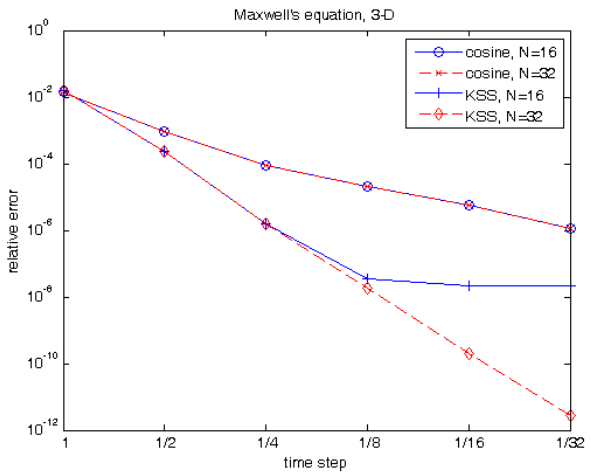

Figure 3: Estimates of relative error at $t = 1$ in solutions of (16), (20) computed using a cosine method based on a Gautschi-type exponential integrator [8, 10] with 2 Lanczos iterations, and a 2-node block KSS method. Both methods compute solutions on an N^3-point grid, with time step Δt, for various values of N and Δt.

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