Krylov Subspace Spectral Methods for Systems of Variable-Coefficient PDE

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Abstract. For scalar time-dependent variable-coefficient PDE, it has been demonstrated that Krylov subspace spectral (KSS) methods achieve high-order accuracy and also possess highly desirable stability properties, especially considering that they are explicit. In this paper, we examine the generalization of these methods to systems of variable-coefficient PDE by selection of appropriate bases of trial and test functions. Furthermore, we show that for certain special cases, even higher-order accuracy is possible, as has previously been established in the case of the scalar second-order wave equation. Finally, we consider the use of KSS methods to obtain high-order operator splittings for systems of equations.

Keywords: Krylov subspace methods, spectral methods, Lanczos algorithm, Gaussian quadrature, variable-coefficient PDE, wave equation
PACS: 02.60.Lj, 02.60.Dc, 02.60.Jh

INTRODUCTION

Consider the initial-boundary value problem in one space dimension,

$$\frac{\partial \mathbf{u}}{\partial t}(x,t) + L(x,D)\mathbf{u}(x,t) = 0, \quad 0 < x < 2\pi, \quad t > 0, \tag{1}$$

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

with periodic boundary conditions

$$\mathbf{u}(0,t) = \mathbf{u}(2\pi,t), \quad t > 0, \tag{3}$$

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

$$L_{ij}(x,D)u(x) = \sum_{\mu=0}^{m_{ij}} a_\mu^{ij}(x) D^\mu u, \quad D = \frac{d}{dx}, \tag{4}$$

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

For the case of $n = 1$, with $L_{11}(x,D)$ a self-adjoint, positive semi-definite operator, a class of methods for numerically solving problems of this form, called Krylov subspace spectral (KSS) methods, was introduced in [1], [2]. These methods achieve high-order accuracy in time, and greater stability than explicit time-stepping methods. In this paper, we discuss how these methods can be generalized to systems of equations.

KRYLOV SUBSPACE SPECTRAL METHODS

Let $n = 1$, in which case $L(x,D)$ is merely a differential operator, which we assume is self-adjoint and positive semi-definite. Then, let $S(x,D;t) = \exp[-L(x,D)t]$ represent the exact solution operator of the problem (1), (2), (3), and let $\langle \cdot, \cdot \rangle$ denote the standard inner product of functions defined on $[0,2\pi]$,

$$\langle f(x), g(x) \rangle = \int_0^{2\pi} \overline{f(x)} g(x)\, dx. \tag{5}$$

KSS methods, introduced in [1], [2], 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 $\tilde{u}(x,t_n)$,

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

KSS methods approximate these components with higher-order temporal accuracy than traditional spectral methods and time-stepping schemes. We briefly review how these methods work.

We discretize functions defined on $[0,2\pi]$ on an N-point uniform grid with spacing $h = 2\pi/N$. With this discretization, the operator $L(x,D)$ and the solution operator $S(x,D;\Delta t)$ can be approximated by $N \times N$ matrices that represent linear operators on the space of grid functions, and the quantity (6) can be approximated by a bilinear form

$$\hat{u}(\omega,t_{n+1}) \approx \hat{\mathbf{e}}_\omega^H S_N(\Delta t)\mathbf{u}(t_n), \tag{7}$$

where

$$[\hat{\mathbf{e}}_\omega]_j = \frac{1}{\sqrt{2\pi}} e^{i\omega jh}, \quad [\mathbf{u}(t_n)]_j = u(jh,t_n), \tag{8}$$

and

$$S_N(t) = \exp[-L_N t], \quad [L_N]_{jk} = \sum_{\mu=0}^{m} a_\mu(jh)[D_N^\mu]_{jk} \tag{9}$$

where D_N is a discretization of the differentiation operator that is defined on the space of grid functions, which are the eigenfunctions of D_N. Our goal is to approximate (7) by computing an approximation to

$$[\hat{\mathbf{u}}^{n+1}]_\omega = \hat{\mathbf{e}}_\omega^H \mathbf{u}(t_{n+1}) = \hat{\mathbf{e}}_\omega^H S_N(\Delta t)\mathbf{u}(t_n). \tag{10}$$

Elements of Functions of Matrices

In [3] Golub and Meurant describe a method for computing quantities of the form

$$\mathbf{u}^T f(A)\mathbf{v} = I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda), \tag{11}$$

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 was defined in (9), $f(\lambda) = \exp(-\lambda t)$ for some t, and the vectors $\mathbf{u}$ and $\mathbf{v}$ are derived from $\hat{\mathbf{e}}_\omega$ and $\mathbf{u}(t_n)$.

Since the matrix A is symmetric positive semi-definite, it has real eigenvalues

$$b = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N = a \geq 0. \tag{12}$$

The measure $\alpha(\lambda)$ is based on the spectral decomposition of A. As discussed in [3], [4], [5], [6], the integral $I[f]$ can be approximated using Gaussian quadrature rules, which yield an approximation of the form

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

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 $\mathbf{u} \neq \mathbf{v}$.

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 [7] for details). Therefore, it is best to handle this case by rewriting (11) using decompositions such as

$$\mathbf{u}^T f(A)\mathbf{v} = \frac{1}{\delta}[\mathbf{u}^T f(A)(\mathbf{u} + \delta\mathbf{v}) - \mathbf{u}^T f(A)\mathbf{u}], \tag{14}$$

where δ is a small constant. Guidelines for choosing an appropriate value for δ can be found in [2, Section 2.2].

Accuracy of KSS Methods

Employing these quadrature rules yields a simple algorithm (for details see [1], [2]) for computing the Fourier coefficients of $\mathbf{u}(t_{n+1})$ from $\mathbf{u}(t_n)$. This algorithm has temporal accuracy $O(\Delta t^{2K})$, so for this reason very few nodes are needed in practice.

This order of accuracy can be compared to the accuracy achieved by an algorithm described by Hochbruck and Lubich in [8] for computing $e^{A\Delta t}\mathbf{v}$ for a given matrix A and vector $\mathbf{v}$ using the unsymmetric Lanczos algorithm. For stiff problems such as (1), (2), (3), time-stepping using this approach yields local temporal error of $O(\Delta t^K)$, assuming a K-dimensional Krylov subspace.

The difference between KSS methods and the approach described in [8] is that in the former, a different K-dimensional Krylov subspace is used for each Fourier component, instead of the same subspace for all components as in the latter. As can be seen from numerical results comparing the two approaches in [2], using the same subspace for all components causes a loss of accuracy as the number of grid points increases, whereas KSS methods do not suffer from this phenomenon.

In [9] it was demonstrated how KSS methods can be applied to problems in higher spatial dimensions with the same accuracy and efficiency as in the one-dimensional case. In this paper, generalizations to systems of equations in higher dimensions will be discussed as well.

GENERALIZATION TO SYSTEMS OF EQUATIONS

Generalization of KSS methods to a system of the form (1) can proceed as follows. For $i, j = 1, \ldots, n$, let $\overline{A}_{ij}(D)$ be the constant-coefficient operator obtained by averaging the coefficients of $A_{ij}(x,D)$ over $[0, 2\pi]$. Then, for each wave number ω, we define $A(\omega)$ be the matrix with entries $\overline{A}_{ij}(\omega)$, i.e., the symbols of $\overline{A}_{ij}(D)$ evaluated at ω.

For simplicity, we assume that $A(\omega)$ is diagonalizable for each ω. For $j = 1, \ldots, n$, let $(\lambda_j(\omega), \mathbf{u}_j(\omega))$ and $(\lambda_j(\omega), \mathbf{v}_j(\omega))$ be right and left eigenpairs, respectively, of $A(\omega)$. Then we define our trial functions by $\mathbf{u}_j(\omega) \otimes e^{i\omega x}$, and our test functions by $\mathbf{v}_j(\omega) \otimes e^{i\omega x}$.

We will show that, as in the scalar case, this approach yields $O(\Delta t^{2K})$ local temporal error. Furthermore, although the quadrature rules described in [3], and employed in KSS methods, were designed for use with self-adjoint positive semi-definite operators, we will demonstrate that the same high-order accuracy can also be achieved with non-self-adjoint differential operators.

Special Cases

In [10], a variation of KSS methods was applied to variable-coefficient, second-order wave equations, achieving $O(\Delta t^{4K})$ accuracy when using a K-node Gaussian rule to approximate each Fourier component. Furthermore, for such problems, Dirichlet boundary conditions were used instead of the periodic conditions that have been imposed throughout this paper, thus demonstrating the suitability of the method for "true" initial-boundary value problems, as opposed to those with periodic boundary conditions. The first-order system to which KSS methods were applied in [10] has the form

$$\begin{bmatrix} u \\ v \end{bmatrix}_t = \begin{bmatrix} 0 & I \\ L(x,D) & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}, \quad u(x,0) = f(x), \quad v(x,0) = g(x), \quad 0 < x < 1, \tag{15}$$

where L is a second-order differential operator, with boundary conditions $u(0,t) = u(1,t) = 0$.

Now, we consider a system of the kind that can arise in the study of acoustics in an inhomogeneous medium,

$$\mathbf{u}_t = A(x,D)\mathbf{u}, \quad 0 < x < 2\pi, \quad t > 0, \tag{16}$$

with

$$\mathbf{u} = \begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}, \quad A(x,D) = \begin{bmatrix} 0 & L_1(x,D) \\ L_2(x,D) & 0 \end{bmatrix}, \tag{17}$$

where $L_1(x,D)$ and $L_2(x,D)$ are first-order differential operators. We include initial conditions

$$u(x,0) = f(x), \quad v(x,0) = g(x), \quad 0 < x < 2\pi, \tag{18}$$

and periodic boundary conditions.

By examination of the Taylor series expansion of $\exp[A(x,D)t]$, we will show that we can approximate the solution by applying a KSS method in which the Lanczos algorithm is applied to the products $L_1(x,D)L_2(x,D)$ and $L_2(x,D)L_1(x,D)$, just as it was applied to $L(x,D)$ in (15). This allows the high-order temporal accuracy of $O(\Delta t^{4K})$ to be achieved for these systems as well.

High-Order Splittings

It is shown in [11] that as $\delta \to 0$ in (14), KSS methods are revealed to be high-order operator splittings "in disguise". In the scalar case, these splittings have the form

$$\exp[-L(x,D)t] = \sum_{k=1}^{K} e^{-C_k(x,D)t}[I - tV_k(x,D)] \tag{19}$$

where K is the number of quadrature nodes, and each operator $C_k(x,D)$ is diagonal in the basis of trial functions (e.g., a constant-coefficient operator when using Fourier series). As shown in [11], these splittings facilitate stability analysis, which demonstrates that KSS methods represent a "best-of-both-worlds" compromise between explicit and explicit time-stepping methods, as they are almost as stable as implicit methods, but like explicit methods, they do not require solution of large systems of equations. This stability analysis will be generalized to cases involving systems of equations.

SUMMARY

We have generalized KSS methods from scalar variable-coefficient time-dependent PDE to systems of such equations by constructing appropriate bases of trial and test functions. This generalization preserves the high-order temporal accuracy that has been achieved in the scalar case. For special cases arising from the second-order wave equation, it is shown that even higher-order accuracy can be achieved, for a wider variety of systems than previously reported, by computing recursion coefficients of appropriately chosen products of differential operators. Finally, it is shown that like their scalar counterparts, KSS methods for systems are equivalent to high-order operator splittings, a perspective which can be used to analyze stability and demonstrate that these methods, while explicit, have stability properties similar to those of implicit methods.

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