Implicitly Defined High-Order Operator Splittings for Parabolic and Hyperbolic Variable-Coefficient PDE Using Modified Moments

James V. Lambers*

September 24, 2008

Abstract

This paper presents a reformulation of Krylov Subspace Spectral (KSS) Methods, which use Gaussian quadrature in the spectral domain compute high-order accurate approximate solutions to variable-coefficient time-dependent PDE. This reformulation reveals that KSS methods are actually high-order operator splittings that are defined implicitly, in terms of derivatives of the nodes and weights of Gaussian quadrature rules with respect to a parameter. We discuss the application of these modified KSS methods to parabolic and hyperbolic PDE, as well as systems of coupled PDE.

1 Introduction

Consider the initial-boundary value problem

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

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

*Department of Energy Resources Engineering, Stanford University, Stanford, CA 94305-2220, USA

with periodic boundary conditions, where $L(x, D)$ is a self-adjoint, positive semi-definite, variable-coefficient differential operator. A class of methods for numerically solving such problems, called Krylov subspace spectral (KSS) methods, was introduced in [5]. These methods achieve high-order accuracy in time, and greater stability than explicit time-stepping methods. However, because these methods approximate derivatives of bilinear forms using finite differences, they are prone to numerical instability. In this paper, we address this issue, and also demonstrate that the resulting modified KSS methods are actually high-order operator splittings.

2 Krylov Subspace Spectral Methods

We discretize functions defined on $[0, 2\pi]$ on an N-point uniform grid with spacing $h = 2\pi/N$, and define $t_n = n\Delta t$ for some time step Δt. With this discretization, the operator $L(x, D)$ can be approximated by an $N \times N$ matrix L_N that represents a linear operator on the space of grid functions, and each Fourier component of the solution can be approximated by a bilinear form

$$\hat{u}(\omega, t_{n+1}) \approx \hat{\mathbf{e}}_\omega^H S_N(\Delta t)\mathbf{u}(t_n), \tag{3}$$

where $[\hat{\mathbf{e}}_\omega]_j = \frac{1}{\sqrt{2\pi}} e^{i\omega jh}$, $[\mathbf{u}(t_n)]_j = u(jh, t_n)$, and $S_N(t) = \exp[-L_N t]$.

In [1] Golub and Meurant describe a method for computing quantities of the form $\mathbf{u}^T f(A)\mathbf{v}$, for a smooth function f, that uses Gaussian quadrature to approximate a Riemann-Stieltjes integral with measure based on the spectral decomposition of the matrix A. The quadrature nodes and weights can be obtained using the Lanczos algorithm. The case $\mathbf{u} \neq \mathbf{v}$ requires the unsymmetric Lanczos algorithm, which is subject to breakdown. This can be avoided by rewriting the bilinear form using decompositions such as

$$\mathbf{u}^T f(A)\mathbf{v} = \frac{1}{\delta}[\mathbf{u}^T f(A)(\mathbf{u} + \delta\mathbf{v}) - \mathbf{u}^T f(A)\mathbf{u}], \tag{4}$$

where δ is a small constant.

Employing these quadrature rules yields a simple algorithm (for details see [5]) 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.

Unfortunately, the difference quotient used to compute each Fourier component of the solution can be numerically unstable if δ is chosen too small, but this parameter must also be chosen small enough to ensure stability of the quadrature rules. We will now address this issue, and realize an additional benefit in the process: operator splittings that are high-order accurate in time, and, though explicit, possess favorable stability properties.

3 Reformulation

For a given δ, let $\lambda_{\omega,j}$ and $w_{\omega,j}$, $j = 1, \ldots, K$, be the nodes and weights of the K-point Gaussian rule obtained by applying the unsymmetric Lanczos algorithm to L_N with starting vectors $\hat{\mathbf{e}}_\omega$ and $(\hat{\mathbf{e}}_\omega + \delta \mathbf{u}^n)$. Then, letting $\delta \to 0$, we obtain

$$[\hat{\mathbf{u}}^{n+1}]_\omega \;=\; \sum_{j=1}^{K} w_{j,\omega} e^{-\lambda_{j,\omega}\Delta t} \left[\hat{\mathbf{e}}_\omega^H \mathbf{u}^n + \frac{w'_{j,\omega}}{w_{j,\omega}} - \Delta t \lambda'_{j,\omega} \right] \qquad (5)$$

where the $'$ denotes differentiation with respect to δ, and evaluation of the derivative at $\delta = 0$. Efficient algorithms for obtaining the derivatives of the nodes and weights are presented in [4].

By considering all Fourier components together, we find that KSS methods are actually high-order operator splittings "in disguise". These splittings have the form

$$\exp[-L\Delta t] \approx \sum_{k=1}^{K} W_k e^{-C_k \Delta t} [I - \Delta t V_k] \qquad (6)$$

where the operators C_k and W_k are diagonal in the basis of trial functions (e.g., a constant-coefficient operator when using Fourier series). In fact, their eigenvalues are the kth nodes and weights, respectively. The operators V_k have the form

$$V_k = C'_k + \Delta t^{-1} W_k^{-1} W'_k \qquad (7)$$

where the Fourier components of $C'_k \mathbf{u}^n$ and $W'_k \mathbf{u}^n$ are the derivatives of the nodes and weights with respect to δ at $\delta = 0$. Because $e^{-C_k \Delta t} \to I$ linearly as $\Delta t \to 0$, and $\sum_{j=1}^{K} W_k = I$, it follows that the terms in V_k of order $O(\Delta t^{-1})$ cancel and pose no difficulty.

As shown in [3], splittings such as this facilitate stability analysis of KSS methods, and such analysis demonstrates that KSS methods represent a "best-of-both-worlds" compromise between implicit and explicit time-stepping methods, as they possess the stability of implicit methods, but like explicit methods, they do not require solution of large systems of equations. However, unlike other splittings in the literature, the stages of the splitting (6) cannot easily be described in terms of the coefficients of L. This is because they are defined in terms of the nodes and weights of quadrature rules, which do not have a simple relation to the recursion coefficients, as they come from the eigenvalues and eigenvectors of Jacobi matrices. Nevertheless, these splittings can still be implemented efficiently, as the action of the operators V_k on a given grid function can be computed from the derivatives of the nodes and weights.

4 Application to the Wave Equation

In this section we consider the problem

$$\frac{\partial^2 u}{\partial t^2} + Lu = 0, \quad (x,t) \in (0, 2\pi) \times \mathbb{R}, \tag{8}$$

with periodic boundary conditions and the initial conditions

$$u(x,0) = f(x), \quad u_t(x,0) = g(x), \quad x \in (0, 2\pi), \tag{9}$$

where the operator L is as described in Section 1.

In [2], KSS methods were applied to this problem. Following the reformulation presented in Section 3 for parabolic problems, we obtain the new time-stepping scheme

$$\begin{aligned}
\begin{bmatrix} \hat{\mathbf{u}}^{n+1} \\ \hat{\mathbf{u}}_t^{n+1} \end{bmatrix}_\omega = &\left(\sum_{k=1}^{K} w_k \begin{bmatrix} c_k & \frac{1}{\sqrt{\lambda_k}} s_k \\ -\sqrt{\lambda_k} s_k & c_k \end{bmatrix} \right) \begin{bmatrix} \hat{\mathbf{u}}^{n} \\ \hat{\mathbf{u}}_t^{n} \end{bmatrix}_\omega + \\
&\sum_{k=1}^{K} \begin{bmatrix} c_k & \frac{1}{\sqrt{\lambda_k}} s_k \\ -\sqrt{\lambda_k} s_k & c_k \end{bmatrix} \begin{bmatrix} w_k' \\ \tilde{w}_k' \end{bmatrix} - \\
&\sum_{k=1}^{K} \frac{w_k t}{2\sqrt{\lambda_k}} \begin{bmatrix} s_k & -\frac{1}{\sqrt{\lambda_k}} c_k \\ \sqrt{\lambda_k} c_k & s_k \end{bmatrix} \begin{bmatrix} \lambda_k' \\ \tilde{\lambda}_k' \end{bmatrix} - \\
&\sum_{k=1}^{K} w_k \begin{bmatrix} 0 & \frac{1}{2(\lambda_k)^{3/2}} s_k \\ \frac{1}{2\sqrt{\lambda_k}} s_k & 0 \end{bmatrix} \begin{bmatrix} \lambda_k' \\ \tilde{\lambda}_k' \end{bmatrix}
\end{aligned}$$

where $c_k = \cos(\sqrt{\lambda_k}t)$, $s_k = \sin(\sqrt{\lambda_k}t)$, and λ'_k and w'_k are the derivatives of the nodes and weights, respectively, in the direction of $\mathbf{u}^n$, while $\tilde{\lambda}'_k$ and $\tilde{w}'_k$ are the derivatives in the direction of $\mathbf{u}^n_t$.

As in the previous section, by considering all Fourier components together, we can write this scheme as a weighted sum of operator splittings. For example, we have the approximation

$$\begin{aligned}\cos(\sqrt{L}\Delta t) \approx \sum_{k=1}^{K} W_k \Big[&\cos(\sqrt{C_k}\Delta t)(I + W_k^{-1}W'_k) - \\ &\frac{1}{2}\Delta t C_k^{-1/2}\sin(\sqrt{C_k}\Delta t)C'_k\Big], \end{aligned} \tag{10}$$

where C_k, W_k, C'_k and W'_k are as defined in Section 3.

As shown in [4], this new formulation has the same order of accuracy as the original presented in [2]. Specifically, the error in each Fourier component is $O(\Delta t^{4K})$, where K is the number of nodes in each Gaussian quadrature rule. Numerical results demonstrating the accuracy, as well as the numerical stability, of reformulated KSS methods for the wave equation are given in [4].

5 Systems of Coupled PDE

In [4], KSS methods were also applied to a system of n coupled variable-coefficient PDE of the form $\mathbf{u}_t + L\mathbf{u}$, where $\mathbf{u} : [0, 2\pi] \times [0, \infty) \to \mathbb{R}^n$ for $n > 1$. The operator L is an $n \times n$ matrix where the (i, j) entry is a differential operator L_{ij}.

Generalization of KSS methods to such a system can proceed as follows. For $i, j = 1, \ldots, n$, let $\overline{L}_{ij}$ be the constant-coefficient operator obtained by averaging the coefficients of L_{ij} over the spatial domain. Then, for each wave number ω, we define $L(\omega)$ to be the matrix with entries equal to the symbols of each $\overline{L}_{ij}$ evaluated at ω. Then, we define our trial and test functions by $\mathbf{q}_j(\omega) \otimes e^{i\omega x}$, where $\mathbf{q}_j$ is a Schur vector of $L(\omega)$.

As in the scalar case, this approach yields $O(\Delta t^{2K})$ local temporal error, where K is the number of nodes in each Gaussian quadrature rule, even though L is not self-adjoint. The recursion coefficients, nodes and weights can be computed in the same manner as in the scalar, self-adjoint case. The result is an implicitly-defined

operator splitting of the form (6). Numerical results presented in [4] demonstrate the effectiveness of KSS methods for such systems.

6 Summary

For both parabolic and hyperbolic variable-coefficient PDE, a reformulation of KSS methods that eliminates the need to perturb quadrature rules reveals that these methods are actually implicitly-defined high-order operator splittings. Although the stages of the splitting are not easily described, efficient algorithms for computing appropriate derivatives of the nodes and weights allow efficient implementation of these methods. We have also shown that KSS methods can also be readily generalized to systems of coupled PDE through an appropriate choice of trial functions.

References

[1] 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)

[2] Guidotti, P., Lambers, J. V., Sølna, K.: Analysis of 1-D Wave Propagation in Inhomogeneous Media. *Numerical Functional Analysis and Optimization* **27** (2006), pp. 25-55.

[3] Lambers, J. V.: Derivation of High-Order Spectral Methods for Time-dependent PDE using Modified Moments. *Electronic Transactions on Numerical Analysis* **28** (2008), pp. 114-135.

[4] Lambers, J. V.: Implicitly Defined High-Order Operator Splittings for Parabolic and Hyperbolic Variable-Coefficient PDE Using Modified Moments. *International Journal of Computational Science* **2** (2008), p. 376-401.

[5] Lambers, J. V.: Krylov Subspace Spectral Methods for Variable-Coefficient Initial-Boundary Value Problems. *Electronic Transactions on Numerical Analysis* **20** (2005), pp. 212-234.