

Recent Advances in Krylov Subspace Spectral Methods

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This paper reviews the main properties, and most recent developments, of Krylov subspace spectral (KSS) methods for time-dependent variable-coefficient PDE. These methods use techniques developed by Golub and Meurant for approximating elements of functions of matrices by Gaussian quadrature in the spectral domain in order to achieve high-order accuracy in time and stability characteristic of implicit time-stepping schemes, even though KSS methods themselves are explicit. In fact, for certain problems, 1-node KSS methods are unconditionally stable. Furthermore, these methods are equivalent to high-order operator splittings, thus offering another perspective for further analysis and enhancement.

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1 Introduction

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

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

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

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 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. We review recent advances in the development of these methods.

2 Krylov Subspace Spectral Methods

Let $S(x, D; t) = \exp[-L(x, D)t]$ represent the exact solution operator of the problem (1), (2). Given the computed solution $\tilde{u}(x, t_n)$ at time t_n , KSS methods compute the solution at time t_{n+1} by approximating the Fourier components that would be obtained by applying the exact solution operator to $\tilde{u}(x, t_n)$. 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 each Fourier component can be approximated by a bilinear form

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

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 $S_N(t) = \exp[-L_N t]$, where L_N is a discretization $L(x, D)$.

In [3] Golub and Meurant describe a method for computing quantities of the form $\mathbf{u}^T f(A) \mathbf{v}$, for a smooth function f , by approximating a Riemann-Stieltjes integral with measure based on the spectral decomposition of the matrix A . The integral can be approximated using Gaussian quadrature rules, where the nodes and weights can be obtained using the Lanczos algorithm. 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 [4] for details). Therefore, it is best to handle this case by rewriting the bilinear form using decompositions such as

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

where δ is a small constant.

3 Properties and Recent Advances

3.1 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.

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This order of accuracy can be compared to the accuracy achieved by an algorithm described by Hochbruck and Lubich in [5] 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), 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 [5] 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 [6] 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.

3.2 High-Order Splittings

It is shown in [7] that as $\delta \rightarrow 0$ in (4), KSS methods are revealed to be high-order operator splittings “in disguise”. These splittings have the form

$$\exp[-L(x, D)t] = \sum_{k=1}^K W_k(x, D)e^{-C_k(x, D)t}[I - tV_k(x, D)] \quad (5)$$

where K is the number of quadrature nodes, and the operators $C_k(x, D)$ and $W_k(x, D)$ are diagonal in the basis of trial functions (e.g., a constant-coefficient operator when using Fourier series), with $\sum_{k=1}^K W_k(x, D) = I$. The operators $V_k(x, D)$ are obtained from directional derivatives of the nodes and weights in the direction of the solution from the previous time step. As shown in [7], 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.

3.3 The Wave Equation

In [8], 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. In [7], it is shown that if the leading coefficient of $L(x, D)$ is constant and the zeroth-order coefficient is sufficiently smooth, a KSS method with $K = 1$ is unconditionally stable, and 2nd-order convergent in time.

4 Summary

For both parabolic and hyperbolic variable-coefficient PDE, KSS methods compute Fourier components of the solution by approximating directional derivatives of moments, where the directions are obtained from the solution from the previous time step. By using the previous solution to perturb Krylov subspaces, rather than generate them, these methods can compute an approximation to each Fourier component that, in some sense, is optimal for that component. As a result, each component is computed with high-order accuracy in time, and, in the case of sufficiently smooth coefficients, unconditional stability is achieved. Therefore, KSS methods represent a viable compromise between the computational efficiency of explicit methods and the stability of implicit methods.

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