Implicitly Defined High-Order Operator Splittings for Time-Dependent Variable-Coefficient PDE Using Modified Moments

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Model Variable-Coefficient Problem

$$\begin{aligned} \frac{\partial u}{\partial t} + L(x, D)u &= 0, \quad 0 < x < 2\pi, \quad t > 0 \\ u(x, 0) &= f(x), \quad 0 < x < 2\pi \\ u(0, t) &= u(2\pi, t), \quad t > 0 \end{aligned}$$

where

$$L(x, D) = -Dp(x)D + q(x), \quad D = \frac{\partial}{\partial x}$$

We assume that $L(x, D)$ is positive semi-definite, and that the coefficients are smooth

Quick-and-Dirty Solution

Let N be an even integer. An approximate solution is

$$\begin{aligned}\tilde{u}(x, t+\Delta t) &= \frac{1}{2\pi}\sum_{\omega=-N/2}^{N/2} e^{i\omega x}\langle e^{i\omega x}, e^{-L(x,D)\Delta t}\tilde{u}(x,t)\rangle \\ &\approx \sum_{\omega=-N/2}^{N/2} e^{i\omega x} e^{-\lambda_\omega \Delta t}\hat{u}(\omega, t)\end{aligned}$$

where $\lambda_\omega = \langle e^{i\omega x}, L(x,D)e^{i\omega x}\rangle$ and $\hat{u}(\omega, t)$ are the coefficients of the Fourier series of $\tilde{u}(x,t)$

This works well if the coefficients of L are nearly constant, but if not, how can we compute $\langle e^{i\omega x}, e^{-L(x,D)\Delta t}\tilde{u}(x,t)\rangle$ as accurately and efficiently as possible?

Elements of Functions of Matrices

If A is $N \times N$ and symmetric, then $u^T e^{-A\Delta t} v$ is given by a Riemann-Stieltjes integral

$$\int_{\lambda_N}^{\lambda_1} e^{-\lambda \Delta t} \, d\alpha(\lambda)$$

where the measure $\alpha(\lambda)$, which is based on the spectral decomposition of A, is positive and increasing if $\mathbf{v} = \mathbf{u}$, or if $\mathbf{v}$ is a small perturbation of $\mathbf{u}$

Gaussian Quadrature

- This integral can be approximated using Gaussian quadrature rules (G. Golub and G. Meurant, '94)
- The nodes and weights are obtained by applying the Lanczos algorithm to A with initial vectors $\mathbf{u}$ and $\mathbf{v}$ to produce T, the tridiagonal matrix of recursion coefficients
- The nodes are the eigenvalues of T, and the weights are obtained from the first components of the left and right eigenvectors
- However, we need to ensure that weights will not be negative

The $\mathbf{u} \neq \mathbf{v}$ Case

For general $\mathbf{u}$ and $\mathbf{v}$, the bilinear form $\mathbf{u}^T e^{-A\Delta t}\mathbf{v}$ can be expressed as the difference quotient

$$\mathbf{u}^T e^{-A\Delta t}\mathbf{v} = \frac{1}{\delta}\left[\mathbf{u}^T e^{-A\Delta t}(\mathbf{u}+\delta\mathbf{v}) - \mathbf{u}^T e^{-A\Delta t}\mathbf{u}\right]$$

where δ is a small constant. Both forms lead to Riemann-Stieltjes integrals with positive, increasing measures

Our goal: to compute Fourier components of the solution by approximating these integrals with $\mathbf{u} = e^{i\omega\mathbf{x}}$, $\mathbf{v} = \tilde{u}(\mathbf{x}, t)$ and A obtained from a discretization of $L(x, D)$

Krylov Subspace Spectral (KSS) Methods[1]

To compute Fourier components of $\tilde{u}(\mathbf{x}, t_{n+1})$, for $n = 0, 1, \ldots$

- Apply symmetric Lanczos algorithm to L with starting vector $e^{i\omega\mathbf{x}}$ to obtain matrix T_ω of recursion coefficients (note: T_ω is a $K \times K$ matrix, where K is the number of quadrature nodes)
- Apply unsymmetric Lanczos algorithm to L with starting vectors $e^{i\omega\mathbf{x}}$ and $e^{i\omega\mathbf{x}} + \delta\tilde{u}(\mathbf{x}, t_n)$ to obtain matrix $T_\omega(\delta)$ of recursion coefficients
- Use eigenvalues and eigenvectors of T_ω and $T_\omega(\delta)$ to approximate, by Gaussian quadrature,

$$\begin{aligned} y_0 &= \langle e^{i\omega\mathbf{x}}, \exp[-L\Delta t]e^{i\omega\mathbf{x}}\rangle, \\ y_\delta &= \langle e^{i\omega\mathbf{x}}, \exp[-L\Delta t](e^{i\omega\mathbf{x}} + \delta\tilde{u}(\mathbf{x}, t_n))\rangle \end{aligned}$$

- Finally, $\hat{u}(\omega, t_{n+1}) = (y_\delta - y_0)/\delta$

[1]See [1]

Computing the Recursion Coefficients

- We need to apply the Lanczos algorithm to a matrix L derived from the operator $L(x, D)$, with two pairs of starting vectors:
  - Case 1: $e^{i\omega \mathbf{x}}$ and $e^{i\omega \mathbf{x}}$
  - Case 2: $e^{i\omega \mathbf{x}}$ and $e^{i\omega \mathbf{x}} + \delta \tilde{u}(\mathbf{x}, t_n)$
- On an N-point grid, this takes $O(N \log N)$ operations for each ω
- Challenge: how to do this in $O(N \log N)$ operations for all ω?
- For case 1, can compute recursion coefficients analytically, as functions of ω
- For case 2, can perturb coefficients from case 1 using $K - 1$ applications of L to $\tilde{u}(\mathbf{x}, t_n)$ and simple recurrence relations (details in [3])

Example

Let $L(x, D) = -Dp(x)D$, and $K = 2$. Then the entries of

$$T_\omega = \begin{bmatrix} \alpha_1 & \beta_1 \\ \beta_1 & \alpha_2 \end{bmatrix}$$

are

$$\begin{aligned} \alpha_1 &= \overline{p}\omega^2 \\ \beta_1^2 &= \overline{p^2}\omega^4 + \overline{[p']^2}\omega^2 - \alpha_1^2 \\ \alpha_2 &= \beta_1^{-2}[\omega^2(\overline{p^3}\omega^4 - 2\overline{p^2 p''}\omega^2 + 4\overline{p(p')^2}\omega^2 + \overline{p(p'')^2}) + 2\alpha_1\beta_1^2 + \alpha_1^3] \end{aligned}$$

where

$$\overline{f} = \frac{1}{2\pi}\int_0^{2\pi} f(x)\,dx$$

Note: these formulas generalize to higher space dimensions

Modifying Recursion Coefficients

This iteration modifies the entries of T_ω to compute

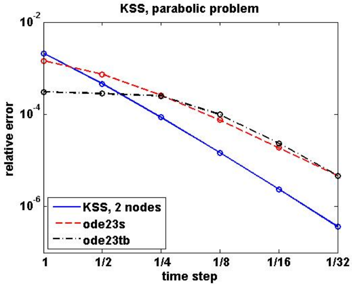
$$T_\omega(\delta) = \begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_1 \\ \hat{\beta}_1 & \hat{\alpha}_2 \end{bmatrix}$$

produced by the unsymmetric Lanczos algorithm applied to L with starting vectors $\mathbf{r}_0$ and $\mathbf{r}_0 + \mathbf{q}_0$, where the $\mathbf{r}_k$ are the unnormalized Lanczos vectors from the symmetric case

In our case, $\mathbf{r}_0 = e^{i\omega\mathbf{x}}$, so inner products with $\mathbf{r}_k$ can be computed simultaneously for all ω using FFTs

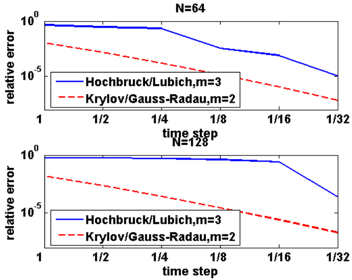
$$\begin{aligned}
\hat{\beta}_0^2 &= \beta_0^2 + \mathbf{r}_0^H \mathbf{q}_0 \\
s_0 &= \frac{\beta_0}{\hat{\beta}_0^2}, \; t_0 = \frac{\beta_0^2}{\hat{\beta}_0^2} \\
\hat{\alpha}_1 &= \alpha_1 + s_0 \mathbf{r}_1^H \mathbf{q}_0 \\
d_1 &= (\alpha_1 - \hat{\alpha}_1) t_0^{1/2} / \hat{\beta}_0 \\
\mathbf{q}_1 &= (L - \hat{\alpha}_1 I)\mathbf{q}_0 \\
\hat{\beta}_1^2 &= t_0 \beta_1^2 + s_0 \mathbf{r}_1^H \mathbf{q}_1 \\
s_1 &= \frac{\beta_1}{\hat{\beta}_1^2} s_0, \; t_1 = \frac{\beta_1^2}{\hat{\beta}_1^2} t_0 \\
\hat{\alpha}_2 &= \alpha_2 + s_1 \mathbf{r}_2^H \mathbf{q}_1 + d_1 \beta_0 t_1^{-1/2}
\end{aligned}$$

Consistency



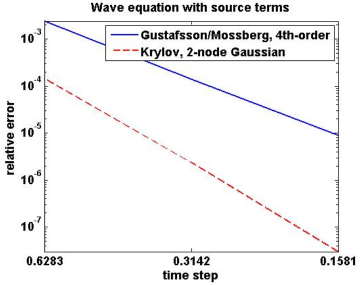
- Gaussian quadrature rules with K nodes are exact for polynomials of degree $2K - 1$ or less
- Quadrature error includes the $2K$-th derivative of the integrand, $e^{-\lambda\Delta t}$
- Therefore, error in each Fourier component is $O(\Delta t^{2K})$!
- Spatial error arises from truncation of Fourier series

Stability



- For parabolic problems, placement of nodes causes damping at higher frequencies (but not too much!)
- Therefore, KSS methods have the stability of implicit methods, even though they are explicit
- Is not restricted by a CFL condition that forces reduction in time step when grid is refined!
- Variation in coefficients, not magnitude, influences stability

The Wave Equation



- The integrands are obtained from the spectral decomposition of the propagator (see [2]):

$$\cos(\sqrt{\lambda}t), \quad \lambda^{\pm 1/2}\sin(\sqrt{\lambda}t)$$

- For each Fourier component, $O(\Delta t^{4K})$ local accuracy!
- For $K = 1$, $p(x)$ constant, $q(x)$ bandlimited, global error is 3rd order in time, and the method is unconditionally stable! (see [4])

In the Limit: Derivatives of Moments!

- Let $T_\omega(\delta)$ be the output of the Lanczos algorithm with starting vectors $e^{i\omega\mathbf{x}}$ and $e^{i\omega\mathbf{x}} + \delta\mathbf{u}^n$, where $\mathbf{u}^n = \tilde{u}(\mathbf{x}, t_n)$
- Each Fourier component of $\mathbf{u}^{n+1}$ approximates the derivative

$$\frac{d}{d\delta}\left[\mathbf{e}_\omega^H(\mathbf{e}_\omega + \delta\mathbf{u}^n)\left(e^{-T_\omega(\delta)t}\right)_{11}\right]_{\delta=0}$$

- Letting $\delta \to 0$ yields

$$[\hat{\mathbf{u}}^{n+1}]_\omega = \sum_{k=1}^{K} w_k e^{-\lambda_k \Delta t}\left([\hat{\mathbf{u}}^n]_\omega + \frac{w_k'}{w_k} - \Delta t \lambda_k'\right)$$

where the λ_k', w_k' are the derivatives of the nodes and weights w.r.t. δ at $\delta = 0$

High-Order Splittings[2]

- Derivatives of nodes and weights w.r.t. δ are Fourier components of applications of pseudodifferential operators applied to $\tilde{u}(\mathbf{x}, t_n)$
- K-node approximate solution has form

$$\tilde{u}(x, t + \Delta t) = \sum_{k=1}^{K} W_k e^{-C_k \Delta t}(I - \Delta t V_k)\tilde{u}(x, t)$$

  where each C_k is a constant-coefficient pseudo-differential operator, of the same order as $L(x, D)$, and positive semi-definite
- Reformulation as splittings facilitates stability analysis
- Unconditionally stable for $K = 1$, solution operator bounded independently of Δt and Δx for $K = 2$

[2] See [5]

Derivatives of the Nodes

There exists a unitary matrix Q_ω^0 such that

$$T_\omega = Q_\omega^0 \Lambda_\omega [Q_\omega^0]^H$$

and the nodes are on the diagonal of Λ_ω. Also,

$$T_\omega(\delta) = Q_\omega(\delta)\Lambda_\omega(\delta)Q_\omega(\delta)^{-1},$$

for suffficiently small δ, where $Q_\omega(0) = Q_\omega^0$

Differentiating with respect to δ and evaluating at $\delta = 0$ yields

$$\mathrm{diag}(\Lambda_\omega') = \mathrm{diag}\left(Q_\omega(0)^H T_\omega' Q_\omega(0)\right),$$

since all other terms arising from differentiation vanish on the diagonal

Derivatives of the Weights

To compute the derivatives of the weights, consider

$$(T_\omega(\delta) - \lambda_j I)\mathbf{w}_j(\delta) = \mathbf{0}, \quad j = 1, \ldots, K,$$

where $\mathbf{w}_j(\delta)$ is a normalized eigenvector of $T_\omega(\delta)$ with eigenvalue λ_j.

- Differentiate with respect to δ, evaluate at $\delta = 0$
- Delete last row and column, using normalization
- We now have a $(K-1) \times (K-1)$ system, where the matrix is tridiagonal plus a rank-one update
- Solve this system, and a similar one for the left eigenvector

We can obtain w_k' from the first components of the two solutions

Derivatives of the Recursion Coefficients

From the expressions for the entries of $T_\omega(\delta)$ in terms of those of T_ω, the derivatives of the recursion coefficients can be obtained by setting $\mathbf{r}_0 = e^{i\omega\mathbf{x}}$ and $\mathbf{q}_0 = \delta\mathbf{u}^n$

By differentiating the recurrence relations with respect to δ and evaluating at $\delta = 0$, we obtain the following algorithm that computes these derivatives

$$[\beta_0^2]' = \mathbf{r}_0^H\mathbf{q}_0$$
$$s_0 = \frac{1}{\beta_0}$$
$$t_0' = -\frac{[\beta_0^2]'}{\beta_0^2}$$
$$d_0' = 0$$

for $j = 1, \dots, K$

$$\alpha_j' = s_{j-1}\mathbf{r}_j^H\mathbf{q}_{j-1} + d_{j-1}'\beta_{j-2}$$

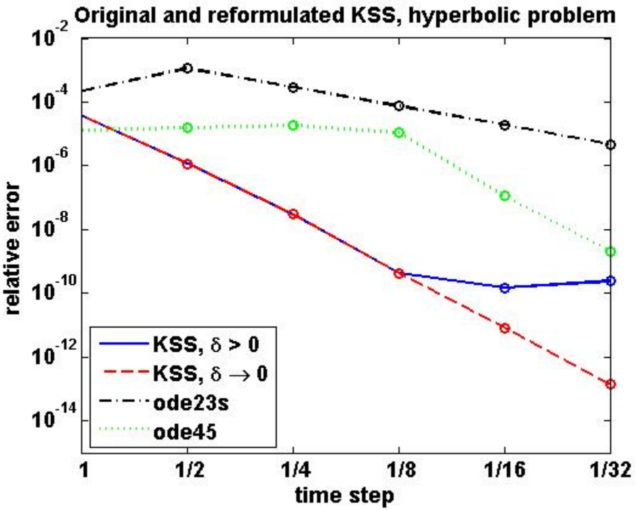
if $j < K$ **then**

$$d_j' = (d_{j-1}'\beta_{j-2} - \alpha_j')/\beta_{j-1}$$
$$\mathbf{q}_j = (L - \alpha_j I)\mathbf{q}_{j-1} - \beta_{j-1}^2\mathbf{q}_{j-2}$$
$$[\beta_j^2]' = t_{j-1}'\beta_j^2 + s_{j-1}\mathbf{r}_j^H\mathbf{q}_j$$
$$s_j = s_{j-1}/\beta_j$$
$$t_j' = t_{j-1}' - \frac{[\beta_j^2]'}{\beta_j^2}$$

end

end

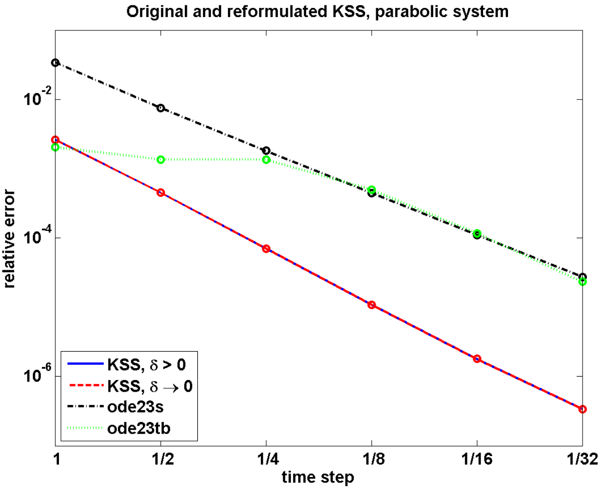
Numerical Stabilization



Systems of Equations

- Generalization to systems of equations is straightforward
- For a system of the form $u_t + A(x, D)u = 0$, where each entry of $A(x, D)$ is a differential operator, we can use trial functions $\mathbf{v}_j \otimes e^{i\omega\mathbf{x}}$ where $\mathbf{v}_j$ is an eigenvector of $\text{Avg}_x A(x, \omega)$
- A corresponding basis of test functions can be used in the same way, except that the left eigenvectors of $\text{Avg}_x A(x, \omega)$ are used instead
- These choices are eigenfunctions of the averaged-coefficient problem

Results


Original and reformulated KSS, parabolic system
relative error
10^-2
10^-4
10^-6
KSS, δ > 0
KSS, δ → 0
ode23s
ode23tb
1
1/2
1/4
1/8
1/16
1/32
time step

Consistency and Stability

- As in the scalar case, a 2-node Gaussian rule yields cubic convergence in time
- Proof is analogous to the scalar case: key is $d^{2K}/d\lambda^{2K}(e^{-\lambda\Delta t}) = (\Delta t)^{2K} e^{-\lambda\Delta t}$ in quadrature error
- Similar stability properties as in scalar case
- However, the Lanczos iteration can break down due to orthogonality of corresponding Lanczos vectors, for example $A(x, D) = [\, 0 \;\; -I; \;\; L(x, D) \; 0 \,]$ where $L(x, D)$ is positive definite

Alternative Bases

- Can use other, orthonormal bases for both trial and test functions
- Instead of using eigenvectors of $\text{Avg}_x A(x, \omega)$, can use Schur vectors, which results in a block diagonalization of the averaged-coefficient operator
- Negligible impact on accuracy, since trial functions are still approximate eigenfunctions
- Fourier coefficients of system components available by solving small orthogonal systems

Time-Dependent Schrödinger Equation

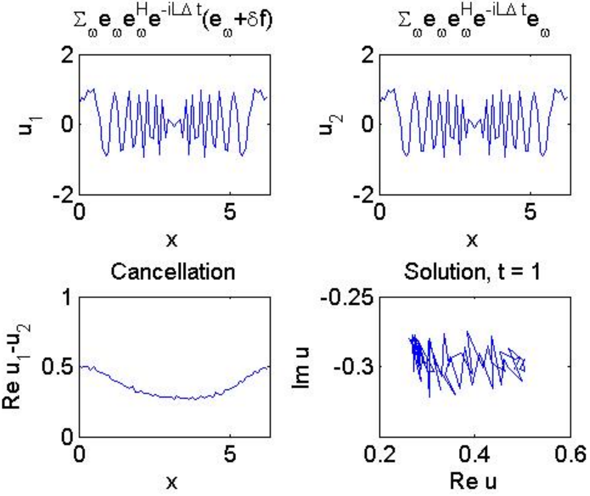
KSS methods can be applied to a problem of the form

$$iu_t = -c\Delta u + Vu$$

simply by using the integrand $e^{-i\lambda\Delta t}$ instead of $e^{-\lambda t}$

The solution has similar smoothness to that of the initial data, but non-smooth or discontinuous coefficients can cause difficulties

Example, Oscillatory Coefficient



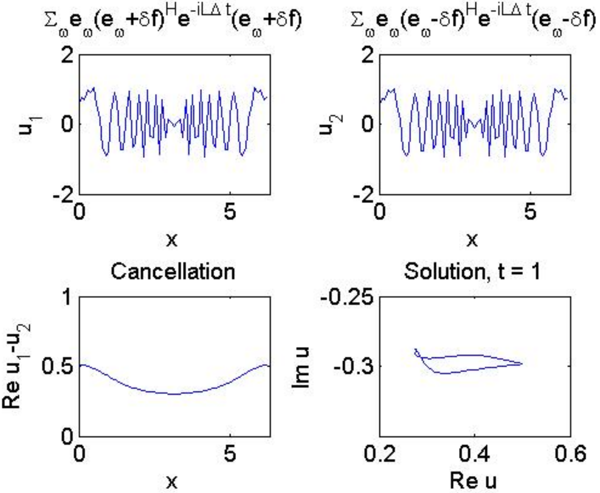
Dealing with Non-Smooth Coefficients

Lack of smoothness in the coefficients can easily be handled by symmetrizing the perturbation, with the polar decomposition

$$\begin{aligned}\mathbf{u}^H e^{-iL\Delta t}\mathbf{v} &= \frac{1}{4}\left[(\mathbf{u}+\mathbf{v})^H e^{-iL\Delta t}(\mathbf{u}+\mathbf{v}) - (\mathbf{u}-\mathbf{v})^H e^{-iL\Delta t}(\mathbf{u}-\mathbf{v})\right] + \\ &\quad \frac{1}{4i}\left[(\mathbf{u}+i\mathbf{v})^H e^{-iL\Delta t}(\mathbf{u}+i\mathbf{v}) - (\mathbf{u}-i\mathbf{v})^H e^{-iL\Delta t}(\mathbf{u}-i\mathbf{v})\right]\end{aligned}$$

If the initial data is not smooth, then $\mathbf{v}$ should be scaled by a parameter δ

Example, Symmetrized Perturbations



Summary and Future Directions

- Krylov subspace spectral methods are showing more promise as their development progresses
  - Applicability to problems with rough behavior, by simply symmetrizing the perturbation!
  - Stability like that of implicit methods
  - Competitive performance and scalability
- Next Steps:
  - Application to other spatial discretizations such as wavelet bases or finite elements
  - Application to more interesting systems of PDE (first results in [5])
  - Generalization of homogenization techniques (see [4]) to higher space dimensions

References

- [1] JL, "Krylov Subspace Spectral Mehods for Variable-Coefficient Initial-Boundary Value Problems", *ETNA* **20** (2005), p. 212-234
- [2] P. Guidotti, JL, K. Sølna, "Analysis of 1-D Wave Propagation in Inhomogeneous Media", *Num. Funct. Anal. Opt.* **27** (2006), p. 25-55
- [3] JL, "Practical Implementation of Krylov Subspace Spectral Methods", *J. Sci. Comput.* **32** (2007), p. 449-476
- [4] JL, "Derivation of High-Order Spectral Methods for Time-Dependent PDE Using Modified Moments", *ETNA* **28** (2008), p. 114-135
- [5] JL, "Implicitly Defined High-Order Operator Splittings for Parabolic and Hyperbolic Variable-Coefficient PDE Using Modified Moments", *Intl. J. Comp. Sci.* (2008), to appear