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Stability of operator splitting methods for systems with indefinite operators: reaction-diffusion systems ☆

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Abstract

In this paper numerical results are reviewed [D.L. Ropp, J.N. Shadid, C.C. Ober, Studies of the accuracy of time integration methods for reaction-diffusion equations, J. Comput. Phys. 194 (2) (2004) 544–574] that demonstrate that common second-order operator-splitting methods can exhibit instabilities when integrating the Brusselator equations out to moderate times of about seven periods of oscillation. These instabilities are manifested as high wave number spatial errors. In this paper, we further analyze this problem, and present a theorem for stability of operator-splitting methods applied to linear reaction-diffusion equations with indefinite reaction terms which controls both low and high wave number instabilities. A corollary shows that if L-stable methods are used for the diffusion term the high wave number instability will be controlled more easily. In the absence of L-stability, an additional time step condition that suppresses the high wave number modes appears to guarantee convergence at the asymptotic order for the operator-splitting method. Numerical results for a model problem confirm this theory, and results for the Brusselator problem agree as well.

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1. Introduction

Operator splitting is a popular method for time integration. Also known as the fractional step method, operator splitting originally developed as a technique for splitting a multi-dimensional spatial operator into a sum of one-dimensional operators in order to simplify the linear algebra [16]. Now it is more commonly used to split different physical terms, such as reaction terms and diffusion terms; see, e.g., [11]. While there are several variations of operator-splitting, here we will focus on first- and second-order methods that split a multiple-term problem into at set of single term equations. The most common second-order operator-splitting methods of this type are those of Strang [14] and Marchuk [9].

In this paper, we focus on systems with indefinite operators. The original non-split systems may be negative definite or indefinite depending on the magnitude of the contribution of the indefinite component operator. This focus was motivated by the observed behavior of numerical solutions of the Brusselator model using these operator-splitting methods. In an earlier study of time integration methods applied to reaction-diffusion systems [13], it was found that when certain second-order operator-splitting methods are used to solve these equations, an instability may arise. This instability is manifested through high wave number oscillations that pollute the solution. This instability persists even when using as many as 1000 time steps per period of oscillation. In contrast, fully implicit methods applied to the full problem are demonstrated to be stable for as few as three time steps per period.

Here, we explore this instability further. We develop theorems that guarantee the stability of these operator-splitting methods applied to certain linear reaction-diffusion equations with indefinite reaction operators. The conditions for stability are simplified if low wave number modes always dominate high wave number modes in the diffusion step, which is the case when the method used for that step is L-stable and monotonic along the negative real axis. These results are demonstrated numerically with a scalar model problem, and are also shown to accurately describe the stability behavior of second-order operator-splitting methods applied to the Brusselator problem.

Stability for operator splitting methods has been studied before in the context of negative definite systems; see, e.g., [3,5,7]. See [6] for a good review of stability results for a variety of operator-splitting methods. In [3] problems of the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = A_1 u + \cdots + A_N u$$

are considered, with $u \in \mathbb{R}^m$ and $A_i \in \mathbb{R}^{m\times m}$, along with the condition that each A_i is negative definite. An operator splitting method then defines an amplification matrix $\mathscr{R}(\Delta t A_1, \ldots, \Delta t A_N)$, and the conditions for A-stability and L-stability are

$$\|\mathscr{R}(\Delta t A_1, \ldots, \Delta t A_N)\| \leqslant 1 \quad \forall \Delta t > 0$$

and

$$\lim_{\Delta t \mu[A_i] \to -\infty} \|\mathscr{R}(\Delta t A_1, \ldots, \Delta t A_N)\| = 0, \quad i = 1, \ldots, N,$$

where $\mu[A_i]$ is the logarithmic norm, defined for a suitable inner product. Here, we use this same definition of A-stability and extend the theory to include systems where one or more of the A_i may be indefinite. We also extend these definitions to the case of an indefinite system.

2. Operator splitting and the Brusselator system

The Brusselator equations, a coupled set of equations first introduced by Prigogine and Lefever [12] as a model of chemical dynamics, are given by

$$\frac{\partial T}{\partial t} = D_1 \frac{\partial^2 T}{\partial x^2} + \alpha - (\beta + 1)T + T^2 C, \tag{1}$$

$$\frac{\partial C}{\partial t} = D_2 \frac{\partial^2 C}{\partial x^2} + \beta T - T^2 C, \tag{2}$$

with the boundary conditions $T(0,t) = T(1,t) = \alpha$ and $C(0,t) = C(1,t) = \frac{\beta}{\alpha}$. Here, T and C represent concentrations of different chemical species. For an explanation of the reaction terms, see [12]. These equations admit steady state, oscillatory and chaotic solutions. In our studies, we consider parameter values of $\alpha = 0.6$, $\beta = 2$, and $D_1 = D_2 = 1/40$, which produce an equilibrium solution with an oscillatory instability. With initial values of $T = \alpha + x(1 - x)$ and $C = \frac{\beta}{\alpha} + x^2(1 - x)$, the resulting solution is oscillatory. We will use a characteristic time scale τ of 12, which is approximately the period of oscillation.

We solve these equations numerically using operator-splitting methods to advance the solution in time. Here, we give an overview of the numerical implementation; for more details see [10,13].

In our implementation of operator splitting we first consider the system as

$$\frac{\mathrm{d}u}{\mathrm{d}t} = F_{\mathrm{D}}(u) + F_{\mathrm{R}}(u), \quad x \in \Omega, \ \ t > 0, \tag{3a}$$

$$u = 0, \quad x \in \partial\Omega, \ \ t > 0. \tag{3b}$$

In the above, u is the vector $[T,C]^{\mathrm{T}}$ and $F_{\mathrm{D}}(u)$ and $F_{\mathrm{R}}(u)$ are the diffusion and reaction terms. We then split the terms, creating two systems of equations. Thus, a single step of a first-order splitting method advancing the solution from t^n to $t^{n+1} = t^n + \Delta t$ amounts to an application of time discretizations applied to the system

$$\frac{\mathrm{d}u^*}{\mathrm{d}t} = F_{\mathrm{R}}(u^*) \quad \text{on } (t^n, t^{n+1}), \qquad u^*(t^n) = u^n, \tag{4a}$$

$$\frac{\mathrm{d}u^{**}}{\mathrm{d}t} = F_{\mathrm{D}}(u^{**}) \quad \text{on } (t^n, t^{n+1}), \qquad u^{**}(t^n) = u^*(t^{n+1}), \tag{4b}$$

with $u^{n+1} = u^{**}(t^{n+1})$. Note that step (4a) has no spatial dependence and thus is essentially an ordinary differential equation (ODE) at each node, requiring no boundary conditions. Step (4b) does have spatial dependence, however, and thus requires application of the boundary conditions stated above.

Using operator notation, we denote the solution of the reaction step as $u^* = S_{\Delta t} u^n$, and the solution of the diffusion step as $u^{**} = D_{\Delta t} u^*$. Thus, the above method can be written as $u^{n+1} = D_{\Delta t} S_{\Delta t} u^n$. We will refer to this method as first-order splitting-diffusion reaction, or FS-DR.

The above operator-splitting method is in general a first-order method. A second-order method can be constructed by taking the above steps over the first half of a time step, and then reversing those steps over the second half of the time step. Using the above notation, this can be written as $u^{n+1} = S_{\Delta t/2} D_{\Delta t} S_{\Delta t/2} u^n$. Known as Strang or Marchuk splitting, we shall refer to it as Strang RDR for reaction-diffusion-reaction.

Within a step of either FS-DR or Strang RDR, we can choose how to integrate the reaction and diffusion steps. Because the reaction step has no explicit spatial dependence, it can be solved as a system of ODEs at each node. These ODEs are time integrated using the CVODE library [1], which implements variable-order (up to 5th-order) BDF methods. The accuracy tolerances are set very low so that the error within the step does not influence the overall error of the splitting method. We allow sub-cycling for the reaction step; that is, within one reaction step of FS-DR or Strang RDR we allow CVODE to take several smaller steps to insure that this step produces a very accurate solution. The diffusion step, solved globally, is integrated using a single step of a one-step method, such as backward Euler or trapezoidal rule.

The spatial discretization is based on a finite element discretization of a Galerkin formulation using a uniform grid of 500 elements with linear basis functions. This results in a system identical to Eq. (4) but with the u, F_R, and F_D replaced by their discretized representations. The discretized representations of F_R and F_D incorporate contributions from the mass matrix of the transient term.

The error that we report here is the ratio of the L_2 norm of the difference of the numerical solution and a reference solution to the L_2 norm of the reference solution. The reference solution is computed using two-point Richardson extrapolation of solutions using a second-order fully-implicit method at the two smallest values of Δt.

3. Preliminary experiments and observations

We first summarize previously reported results. Fig. 1 shows the norm of the error of the solutions at $t = 80 \approx 6.7\tau$. Results are shown for FS-DR using backward Euler for the diffusion term, Strang RDR using trapezoidal rule for the diffusion term, and trapezoidal rule for the fully coupled system. Both FS-DR and trapezoidal rule have good convergence for the entire range of Δt at their expected rates of convergence. For Strang RDR, however, there is no convergence unless Δt is sufficiently small. For Δt small enough, the convergence is second-order as expected and the error is almost two orders of magnitude less than that of trapezoidal rule.

In fact if we look at the solution using Strang RDR we see that high wave number oscillations have polluted the solution, suggesting an instability. This is seen in Fig. 2, which plots the solution using Strang RDR with $\Delta t = 1.6 = 0.13\tau$ at $t = 32$ against a reference solution at this time. This behavior has been discussed previously in [13]. Here, we note that we need to use nearly 1000 time steps per period in order to get acceptable accuracy and convergence. This is very restrictive, and suggests a fundamental problem in using this method to solve this system of equations. In addition, as demonstrated in [13], these methods exhibit

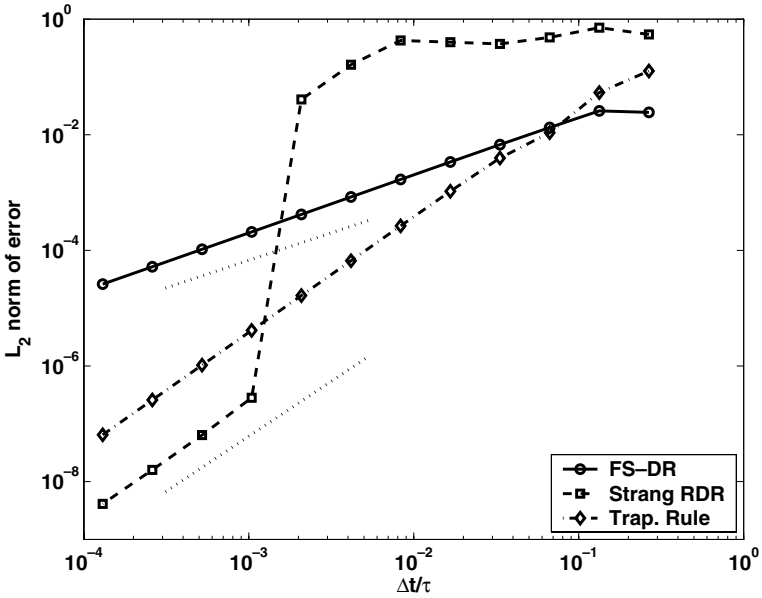

Fig. 1. Temporal convergence FS-DR, Strang RDR, and trapezoidal at $t = 80 \approx 6.7\tau$ ($\tau = 12$). The dotted lines are references with first- and second-order slopes.

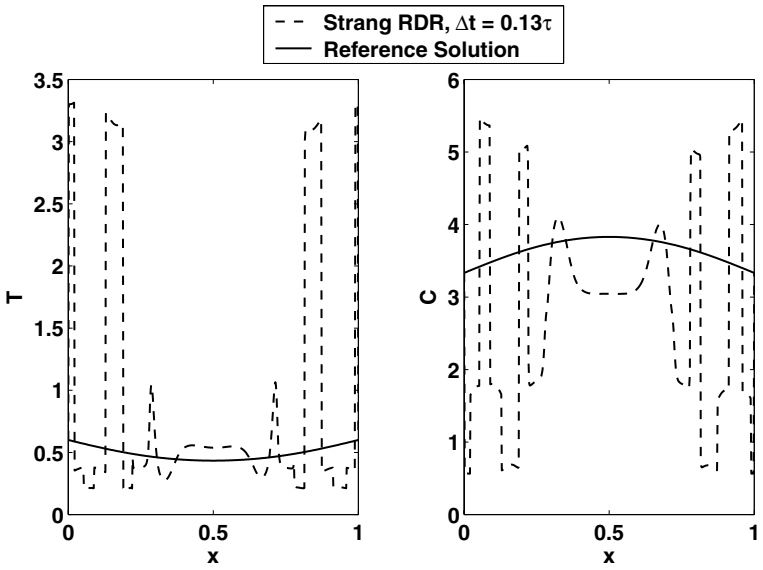

Fig. 2. Solution using Strang RDR with $\Delta t = 1.6 \approx 0.13\tau$ at $t = 32 \approx 2.7\tau$ ($\tau = 12$). The reference solution at this time is also plotted.

very disturbing convergence behavior when both spatial and temporal discretizations are considered. For example, for a fixed time step, decreasing the mesh spacing can cause an increase in the error at moderate integration times of 6.7τ.

This instability was also observed in [15], in which a model of chemotaxis was studied. This paper did not come to the attention of the authors until after the first draft of the current paper, so that model is not examined here.

If we compare the operator forms of FS-DR and Strang RDR, we have for FS-DR

$$u^n = S_{\Delta t} D_{\Delta t} u^{n-1} = S_{\Delta t} D_{\Delta t} \cdots S_{\Delta t} D_{\Delta t} u^0 = (S_{\Delta t} D_{\Delta t})^n u^0,$$

while for Strang RDR we have

$$u^n = S_{\Delta t/2} D_{\Delta t} S_{\Delta t/2} u^{n-1} = S_{\Delta t/2} D_{\Delta t} S_{\Delta t} D_{\Delta t} \cdots D_{\Delta t} S_{\Delta t/2} u^0 = S_{\Delta t/2} D_{\Delta t} (S_{\Delta t} D_{\Delta t})^{n-1} S_{\Delta t/2} u^0.$$

Thus, with the exception of their starting and stopping steps, the order and frequency of the split steps are equivalent for these two methods. We therefore heuristically conclude that any difference in stability between the FS-DR and Strang RDR methods is due to differences in stability of the methods used for the split steps. Since the reaction steps are all solved with the same method, we suspect that the stability of FS-DR is due to the backward Euler method's strong damping of high wave number modes in the diffusion step. Similarly, the instability of Strang RDR may be due to the trapezoidal rule's poor damping of high wave number modes. Indeed, though not shown here, FS-DR is unstable if the trapezoidal rule is used for diffusion, while Strang RDR is stable if backward Euler is used for diffusion. We analyze the FS-DR method further in Section 4.

4. Stability of operator-splitting methods: A-stability

The definitions of stability we use here consider the linear system

$$\frac{du}{dt} = \lambda, \quad u(0) = u_0, \tag{5}$$

where λ is a complex constant. After temporal discretization using a one-step method, this equation becomes a difference equation of the form

$$u^{n+1} = \mathscr{R}(\Delta t\lambda)u^n, \quad u^0 = u_0.$$

Here, $\mathscr{R}(\Delta t\lambda)$, called the amplification factor, is determined by the method and is typically a rational polynomial approximation of $e^{\Delta t\lambda}$. For example, the amplification factors for the backward Euler and trapezoidal rule methods are

$$\mathscr{R}_{\mathrm{BE}}(z) = [1-z]^{-1},$$
$$\mathscr{R}_{\mathrm{TR}}(z) = \left[1-\frac{z}{2}\right]^{-1}\left[1+\frac{z}{2}z\right].$$

The scheme is considered absolutely stable, or A-stable, at a value $z \in \mathbb{C}$ if $|\mathscr{R}(z)| \leqslant 1$. The set of values of z in the complex plane for which this is true is called the A-stability region. In particular, a method is said to be A-stable if its stability region includes the left half-plane, i.e., if $|\mathscr{R}(z)| \leqslant 1$ whenever $\mathrm{Re}(z) \leqslant 0$. This ensures that, when using this method, modes in the numerical solution will decay when the corresponding modes in the original problem decay analytically. Examining the above amplification factors for backward Euler and trapezoidal rule shows that both of these methods are A-stable. See, e.g., [8] for further discussion.

Another useful stability concept is that of L-stability. Sometimes known as strong A-stability or stiff A-stability, L-stability requires A-stability and the condition that $\lim_{z\to-\infty}\mathscr{R}(z) = 0$. This ensures that the $\mathscr{R}$ has the correct asymptotic behavior in the limit of large negative z. The backward Euler method is L-stable, but the trapezoidal rule is not. In fact it is well known that $\lim_{z\to-\infty}\mathscr{R}(z) = -1$ for trapezoidal rule and unphysical high wave number modes decay slowly.

We study the stability of a split system such as Eq. (4) similarly. We assume Eq. (3) represents a system that has been spatially discretized, and that the reaction and diffusion terms are linear, with $F_\alpha(u) = A_\alpha u$, $\alpha = D,R$. Then Eq. (3) is written as

$$\frac{\mathrm{d}u}{\mathrm{d}t} = A_{\mathrm{D}}u + A_{\mathrm{R}}u, \quad x \in \Omega, \ \ t > 0, \tag{6a}$$

$$u = 0, \quad x \in \partial\Omega, \ \ t > 0, \tag{6b}$$

where $u \in \mathbb{R}^N$ and $A_{\mathrm{D}}, A_{\mathrm{R}} \in \mathbb{R}^{N\times N}$. Using FS-DR with solution methods $S_{\Delta t} = \mathscr{R}_{\mathrm{R}}(\Delta t A_{\mathrm{R}})$ and $D_{\Delta t} = \mathscr{R}_{\mathrm{D}}(\Delta t A_{\mathrm{D}})$, our discretized system is

$$\begin{aligned} u^* &= \mathscr{R}_{\mathrm{R}}(\Delta t A_{\mathrm{R}})u^n, \\ u^{n+1} &= \mathscr{R}_{\mathrm{D}}(\Delta t A_{\mathrm{D}})u^*, \end{aligned} \tag{7}$$

with u^{n+1} satisfying the boundary condition. Eliminating u^* gives

$$u^{n+1} = \mathscr{R}_{\mathrm{D}}(\Delta t A_{\mathrm{D}})\mathscr{R}_{\mathrm{R}}(\Delta t A_{\mathrm{R}})u^n$$

or

$$u^{n+1} = \mathscr{R}_{\mathrm{FS-DR}}(\Delta t A_{\mathrm{D}}, \Delta t A_{\mathrm{R}})u^n,$$

where $\mathscr{R}_{\mathrm{FS-DR}}(\Delta t A_{\mathrm{D}}, \Delta t A_{\mathrm{R}}) = \mathscr{R}_{\mathrm{D}}(\Delta t A_{\mathrm{D}})\mathscr{R}_{\mathrm{R}}(\Delta t A_{\mathrm{R}})$. The condition for A-stability is similar to that for the scalar ODE above:

$$\|\mathscr{R}_{\mathrm{FS-DR}}(\Delta t A_{\mathrm{D}}, \Delta t A_{\mathrm{R}})\| \leqslant 1, \quad 0 < \Delta t \leqslant \Delta t^*. \tag{8}$$

Here, Δt^* is the time step limit due to stability. The A-stability criteria for other operator-splitting methods such as Strang and Marchuk is similar. Results of split schemes when A_{D} and A_{R} are negative definite can be found in [3,5].

We are interested initially in A-stability for FS-DR, so we assume that $A_D + A_R$ is negative definite. For the systems we consider that the matrix A_D is a discrete representation of a diffusion operator and thus is also negative definite with a complete set of eigenvectors $\{\phi_i\}_i^N$ with real negative eigenvalues $\lambda_N \leqslant \cdots \leqslant \lambda_1 \leqslant 0$. This is the case, in particular, if A_D arises from a finite element discretization of a linear diffusion operator with Dirichlet boundary conditions.

We do not make any assumption about the reaction term, however, except that $A_D + A_R$ is negative definite. Thus, A_R may have eigenvalues with positive real part, so that the solution grows during the reaction step. In practice this step is solved with an ODE integrator that is sub-cycled with very strict accuracy tolerances, so it is reasonable to assume the step is solved exactly. The following theorem shows the time step restrictions required for the FS-DR method to be A-stable.

Theorem 1. *Let Eq. (7) be an operator-split time-discretization of Eq. (6). Assume that*

- $A_D + A_R$ is negative definite;
- A_D is normal with real negative eigenvalues, with $\lambda_n \leqslant \cdots \leqslant \lambda_1 < 0$;

Let $v_R(\Delta t) = \|\mathscr{R}(\Delta t A_R)\|_{L_2}$. *If the following condition holds*:

$$\max_i |\mathscr{R}_D(\Delta t \lambda_i)| \leqslant 1/v_R(\Delta t) \quad \text{for } 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty, \tag{9}$$

then the operator splitting method given by Eq. (7) is stable, in the sense that Condition (8) is satisfied.

Proof. Because A_D is normal, $\mathscr{R}_D(\Delta t A_D)$ is also normal and

$$\|\mathscr{R}_D(\Delta t A_D)\|_{L_2} = \max_i |\mathscr{R}_D(\Delta t \lambda_i)|.$$

Using Condition (9) with this relation guarantees

$$\|\mathscr{R}_D(\Delta t A_D)\|_{L_2} \leqslant 1/v_R(\Delta t).$$

This gives

$$\|\mathscr{R}_{FS-DR}(\Delta t A_D, \Delta t A_R)\|_{L_2} \leqslant \|\mathscr{R}_D(\Delta t A_D)\|_{L_2} \|\mathscr{R}(\Delta t A_R)\|_{L_2} \leqslant 1.$$

Hence, this splitting method is stable. □

The situation simplifies if $\mathscr{R}_D$ is monotonically increasing on $(-\infty, 0)$, which is the case for many A-stable methods such as backward Euler and trapezoidal rule, and even more so if $\mathscr{R}_D$ is L-stable. Considering these simplifications, we have

Corollary 1. *If* $\mathscr{R}_D$ *is monotonically increasing on* $(-\infty, 0)$, *then Condition (9) can be replaced by*

$$\max(|\mathscr{R}_D(\Delta t \lambda_1)|, |\mathscr{R}_D(\Delta t \lambda_n)|) \leqslant 1/v_R(\Delta t) \quad \text{for } 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty. \tag{10}$$

If $\mathscr{R}_D$ *is also L-stable, then Condition (10) simplifies to*

$$|\mathscr{R}_D(\Delta t \lambda_1)| \leqslant 1/v_R(\Delta t) \quad \text{for } 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty. \tag{11}$$

Proof. By the monotonicity of $\mathscr{R}_D(z)$, we have that for all j,

$$\mathscr{R}_D(\Delta t \lambda_n) \leqslant \mathscr{R}_D(\Delta t \lambda_j) \leqslant \mathscr{R}_D(\Delta t \lambda_1),$$

so

$$\max_j |\mathscr{R}_D(\Delta t \lambda_j)| = \max(|\mathscr{R}_D(\Delta t \lambda_1)|, |\mathscr{R}_D(\Delta t \lambda_n)|).$$

Thus, Condition (10) ensures that Condition (9) is satisfied.

If $\mathscr{R}_D$ is also L-stable, then by its monotonicity and Condition (11) we have

$$0 \leqslant \mathscr{R}_D(\Delta t\lambda_n) \leqslant \mathscr{R}_D(\Delta t\lambda_1) \leqslant 1/\nu_R(\Delta t).$$

Thus, Condition (11) ensures Condition (10) is satisfied and that the method is stable. □

An additional advantage with L-stable methods such as backward Euler is that, in the case where A_D is a discretization of the diffusion operator, Condition (11) can often be satisfied with a Δt^* that is independent of the spatial discretization. For methods that are not L-stable, Condition (10) will not be independent of the spatial discretization in general, however.

For Strang RDR, a similar analysis yields an amplification factor of

$$\mathscr{R}_{\text{Strang RDR}} = \mathscr{R}_R\left(\frac{\Delta t}{2}A_R\right)\mathscr{R}_D(\Delta t A_D)\mathscr{R}_R\left(\frac{\Delta t}{2}A_R\right).$$

The amplification factor from the diffusion step appears in $\mathscr{R}_{\text{Strang RDR}}$ in a similar manner as in $\mathscr{R}_{\text{FS-DR}}$. Thus, the analysis for Strang RDR proceeds exactly as that for FS-DR.

We briefly discuss some terminology. The stability analysis above is for linear problems. In this context, if the stability criteria are violated the numerical solution will experience unbounded growth. Hence, we refer to this behavior as an instability. In the case of a nonlinear system growth can be modulated and restricted. This modulated growth can lead to the appearance of spurious modes in the solution.

Though not shown here, other operator-splitting methods exhibit instabilities similar to those of Strang splitting, such as Romero splitting (see [13]) and Peaceman–Rachford. For each of these methods, though, the contribution to the amplification factor due to the diffusion operator can be viewed as being identical to the contribution $\mathscr{R}_D$ to $\mathscr{R}_{\text{FS-DR}}$ above when using trapezoidal rule for the diffusion. Consequently, these methods have similar difficulties in damping out high wave number modes.

5. An amplification factor spectral decay condition

While Condition (9) ensures A-stability of FS-DR, we have no information about the order of convergence of the method. Moreover, Theorem 1 does not require that the amplification factor for the diffusion solver has the correct asymptotic behavior. This could result in a solution where all the modes are stable but with high wave number modes dominating the low wave number modes. This motivates the following condition:

A Spectral Decay Condition. In addition to the conditions of Theorem 1, we also impose a time step limit $\widetilde{\Delta t}$ such that the following condition holds:

$$\max_i |\mathscr{R}_D(\Delta t\lambda_i)| = \mathscr{R}_D(\Delta t\lambda_1), \quad 0 < \Delta t \leqslant \widetilde{\Delta t}. \tag{12}$$

If $\mathscr{R}_D$ is monotonic then this condition becomes

$$|\mathscr{R}_D(\Delta t\lambda_n)| \leqslant \mathscr{R}_D(\Delta t\lambda_1), \quad 0 < \Delta t \leqslant \widetilde{\Delta t}. \tag{13}$$

If $\mathscr{R}_D$ is monotonic and L-stable, then Condition (12) is automatically satisfied.

While this condition is not necessary for the stability of the operator-splitting method, it does ensure that the low wave number mode is damped the least, which is the behavior of the exact solution of the diffusion

step. Also, the highest wave number modes in a discretized problem often correspond to numerical error, so it is reasonable that these modes should be damped more than the low wave number modes.

Let us also consider the order of convergence. Assume that $\mathscr{R}_D$ is consistent of order $p \geqslant 1$, i.e.,

$$\mathscr{R}_D(z) = e^z + \rho_D(z),$$

where $\rho_D(z) = \mathscr{O}(z^{p+1})$ as $z \to 0$. If Condition (12) holds, then we have

$$\|\mathscr{R}_D(\Delta t A_D)\| = \max_i |\mathscr{R}_D(\Delta t \lambda_i)| = \mathscr{R}_D(\Delta t \lambda_1) = e^{\Delta t \lambda_1} + \rho_D(\Delta t \lambda_1),$$

where we assume that $\Delta t \lambda_1$ small enough that the above expansion holds. Thus, for our implementation of FS-DR, assuming that the reaction step is solved exactly, we have

$$\|u^{n+1}\| \leqslant \|\mathscr{R}_D(\Delta t A_D)\mathscr{R}_R(\Delta t A_R)u^n\| = \mathscr{R}_D(\Delta t \lambda_1)\left\|e^{\Delta t A_R}\right\|\|u^n\| = e^{\Delta t \lambda_1}\left\|e^{\Delta t A_R}\right\|\|u^n\| + \rho_D(\Delta t \lambda_1)\left\|e^{\Delta t A_R}\right\|\|u^n\|.$$

If u^n is composed primarily of low wave number modes, then the term on the left will be a good approximation of the solution using FS-DR with exact component operators. Because $|\lambda_1|$ is not large, the second term on the right side is $\mathscr{O}(\Delta t^{p+1})$. By this heuristic argument, we expect that the numerical solution will exhibit its asymptotic rate of convergence if Condition (12) is satisfied.

6. A simple demonstration of A-stability theorem

We demonstrate the restrictions of Theorem 1 with a model problem, using FS-DR splitting, solving the diffusion step with a single step of either backward Euler (FS-D_{BE}R), trapezoidal rule (FS-D_{TR}R), or one of two SDIRK methods (FS-D_{S1}R and FS-D_{S2}R). The SDIRK, or singly diagonally implicit Runge–Kutta, methods, more fully explained in the Section 8, are a family of implicit Runge–Kutta methods, with S1 being second-order and L-stable and S2 being third-order and A-stable but not L-stable, both with amplification factors which are monotonically increasing on $(-\infty, 0)$. Based on the analysis of the previous section, we expect that operator-splitting methods will be stable as long as Condition (10) is satisfied.

We consider a linear scalar equation and demonstrate the consequences of the conditions of Theorem 1. The equation is

$$u_t = u_{xx} + \alpha u, \quad x \in [0,1], \ \ t > 0, \tag{14}$$

with the boundary conditions $u(x = 0) = u(x = 1) = 0$ and the initial condition $u(t = 0) = 4x * (1 - x)$. The largest eigenvalue of the diffusion operator on this domain is $-\pi^2$, so if $\alpha < \pi^2$ the solution of this problem will decay to 0. Initially we set $\alpha = 8$.

We split this equation using FS-DR. The reaction term is solved exactly as an ODE at each node. For the diffusion term we use linear finite elements for the spatial discretization, with an element size of $\Delta x = 0.1$. This results in a coupled system of linear equations

$$u_t = M^{-1}Ku,$$

with K being the discrete representation of the diffusion operator and M being the mass matrix. For this discretization, the smallest and largest eigenvalues of $M^{-1}K$ are $\lambda_1 = -9.951$ and $\lambda_N = -1116$. We integrate this system using a single step of backward Euler, trapezoidal rule, or one of the SDIRK methods.

We can graphically demonstrate the conditions for stability. In Fig. 3, we plot $1/\|\mathscr{R}(\Delta t A_R)\| = \exp(-8\Delta t)$ and $\mathscr{R}_D(\Delta t \lambda_i)$ for the various methods. To check Condition (10), we need to determine Δt^* such that the plots of $\mathscr{R}_D(\lambda_1 \Delta t)$ and $\mathscr{R}_D(\lambda_N \Delta t)$ are below the plot of $e^{-8\Delta t}$ for $\Delta t \leqslant \Delta t^*$. For backward Euler and SDIRK-1, because these methods are L-stable we only need to check Condition (11). We see that this will hold for $\Delta t^* \approx 0.053$ for backward Euler and $\Delta t^* \approx 0.082$. for SDIRK-1. Moreover, because these methods are L-stable, the spectral decay condition (12) is satisfied.

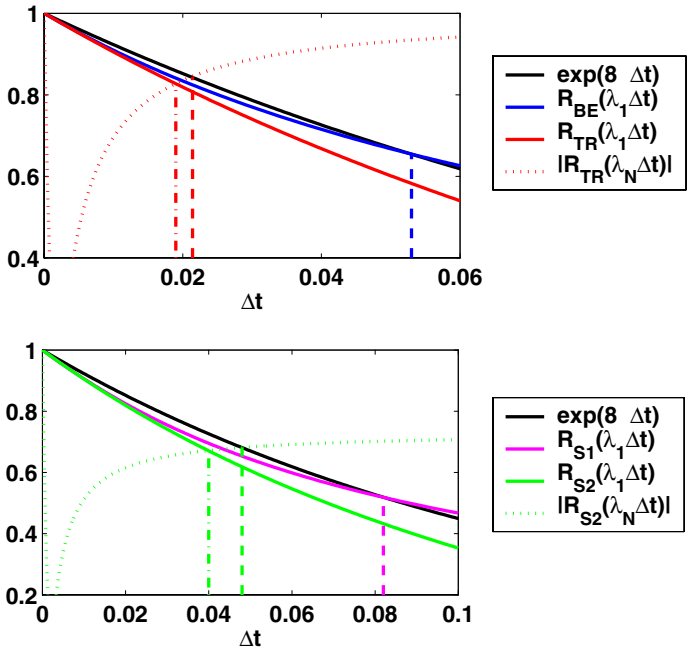

Fig. 3. Amplification factors for the diffusion terms compared to the reciprocal of the amplification factor for the reaction term. Dashed lines indicate values of Δt^* while dash-dot lines indicate values of $\widetilde{\Delta t}$.

For the trapezoidal rule and SDIRK-2, we see that Condition (10) is violated with $\mathscr{R}_D(\lambda_N \Delta t)$, at $\Delta t^* = 0.021$ for trapezoidal rule and $\Delta t^* = 0.048$ for SDIRK-2. The low wave number mode does not violate Condition (10) for these methods. While these restrictions will allow these methods to be stable, to satisfy the spectral decay condition (12) we would require the stricter conditions $\Delta t \leqslant 0.019$ for trapezoidal rule and $\Delta t \leqslant 0.040$ for SDIRK-2. For this problem these values of $\widetilde{\Delta t}$ are close enough to Δt^* that we do not make a distinction between them.

In Fig. 4 a convergence study is presented for the model equation. We integrate this problem from $t = 0$ to $t = 2$ using time steps ranging from $\Delta t = 0.2$ to $\Delta t = 0.003125$, and compute the error with respect to a reference solution based on a Richardson's extrapolation of the two solutions using FS-DR with trapezoidal rule with the smallest Δt. Note that the reaction and diffusion operators for this problem commute, so for small Δt the FS-D_{TR}R and FS-D_{S1}R methods have second-order convergence, while the FS-D_{S2}R method has third-order convergence.

As with the Brusselator problem, for FS-D_{TR}R there is a noticeable transition in the error. For $\Delta t \leqslant 0.02$ the error is small and the solution has the expected second-order convergence. For larger Δt, the error is large. This transition is also seen in FS-D_{S2}R for $\Delta t > 0.05$, as expected. For FS-D_{BE}R and FS-D_{S1}R the error for large enough Δt is large, but there is no clear transition.

The reason for this can be seen in Fig. 5, where we plot the product of the amplification factors of the reaction and diffusion steps. For the FS-D_{BE}R and FS-D_{S1}R this product gradually changes from having slight damping to having growth. The growth of the numerical solution, roughly $\max_i \mathscr{R}_D(\lambda_i \Delta t) \times \exp(8\Delta t)$, is a smooth function. However, for FS-D_{TR}R and FS-D_{S2}R this product initially decays with increasing Δt but then abruptly starts to increase with increasing Δt.

Fig. 6 shows the behavior of the numerical solution for using FS-D_{BE}R and FS-D_{TR}R with different time steps. For both FS-D_{BE}R and FS-D_{TR}R, if $\Delta t < \Delta t^*$, as in (b) and (d), the solution has the correct behavior of damping, though the damping occurs at different rates. For FS-D_{TR}R, if $\Delta t > \Delta t^*$, as in (c), the low wave

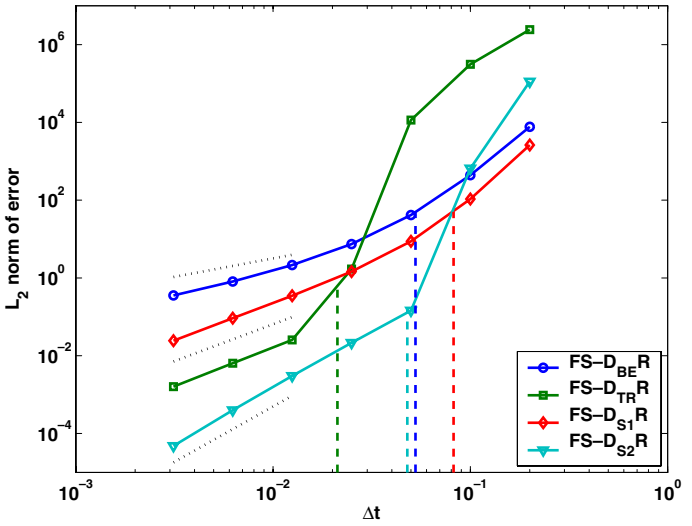

Fig. 4. L_2 error of the solution of Eq. (14). The dashed lines indicate the value of Δt^* for each method. The dotted lines are references with first-, second-, and third-order slopes.

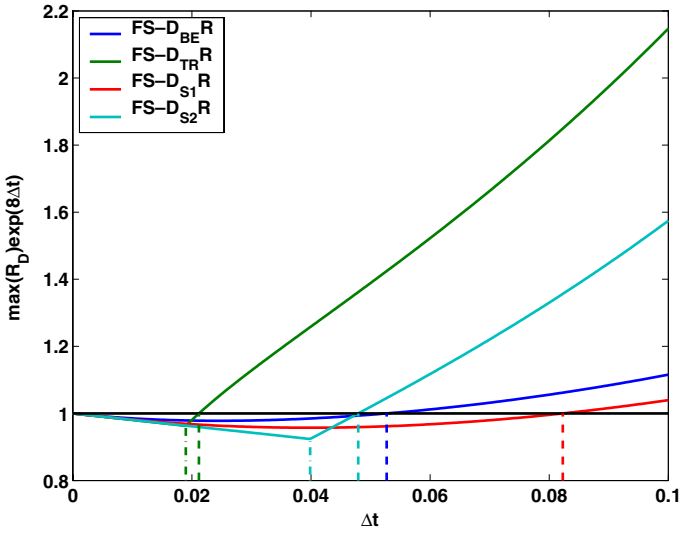

Fig. 5. Product of the maximum amplification factor for the diffusion term and the amplification factor for the reaction term. Methods are unstable when this ratio is greater than 1. Dashed lines indicate the value of Δt^*, while dash-dot lines indicate the value of $\widetilde{\Delta t}$.

number mode damps, but the high wave number modes grow quickly. For FS-D_{BE}R, if $\Delta t > \Delta t^*$, as in (a), the low wave number mode actually grows. Because the solution stays smooth it still looks "realistic" and this instability may not be detected.

In general, Condition (9) or Condition (10) is difficult to check, much less determine a priori. Even for this simplified test case we use graphical means to check them rather than solve the transcendental equations to which they give rise. We can make some useful observations from this test case, though. If Condition (10) is violated with low wave number modes, the solution changes gradually from a low wave number solution that damps to one that grows, and may appear to be physically correct. If Condition

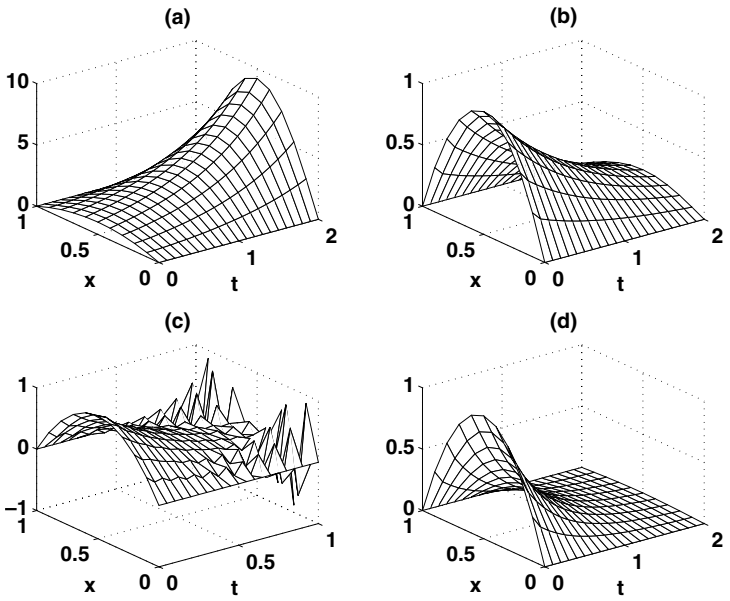

Fig. 6. Profile of the solution using different time steps and different methods for the diffusion step: (a) FS-$D_{BE}R$, $\Delta t = 0.1 \approx 0.0083\tau$; (b) FS-$D_{BE}R$, $\Delta t = 0.025 \approx 0.0021\tau$; (c) FS-$D_{TR}R$, $\Delta t = 0.05 \approx 0.0042\tau$; (d) FS-$D_{TR}R$, $\Delta t = 0.0125 \approx 0.0010\tau$ ($\tau = 12$). Note the change of scales in (a) and (c).

(10) is violated with high wave number modes, the plot of the error will show an abrupt transition from good convergence with low error to poor or no convergence with high error.

We have not made any explicit connection of Δt^* to the spatial discretization. We have only assumed that the spatial discretization is at a fine enough resolution so that the eigenvalues of $A_D + A_R$ are in the left half-plane. For the model problem this is the case; indeed, the largest and smallest eigenvalues of A_D are

$$\lambda_1 = -\frac{6}{\Delta x^2}\left(\frac{1-\cos(\pi\Delta x)}{2+\cos(\pi\Delta x)}\right) \approx -\pi^2\left(1-\frac{\pi^2\Delta x^2}{12}\right)$$

and

$$\lambda_n = -\frac{6}{\Delta x^2}\left(\frac{1+\cos(\pi\Delta x)}{2-\cos(\pi\Delta x)}\right) \approx -\frac{12}{\Delta x^2}\left(1-\frac{3\pi^2\Delta x^2}{4}\right).$$

Using this approximation for λ_1 and evaluating Condition (11) for backward Euler we have that in the limit as $\Delta x \to 0$, $\Delta t^* \approx 0.0507$, with no dependence on Δx. For trapezoidal rule, however, using this approximation for λ_n and evaluating Condition (10) gives $\widetilde{\Delta t^*} \approx \Delta x/2\sqrt{6}$ in the limit as $\Delta x \to 0$.

For the choice of $\alpha = 8$, the values of Δt^* and $\widetilde{\Delta t}$ for FS-$D_{TR}R$ and FS-$D_{S2}R$ are close together. To see more of a distinction between $\widetilde{\Delta t}$ and Δt^*, we consider the same problem but with $\alpha = 1$. Now the solution is strongly damped and the range of Δt for which FS-DR is A-stable is greater. The values of Δt^* for FS-$D_{BE}R$, FS-$D_{TR}R$, FS-$D_{S1}R$, and FS-$D_{S2}R$ are 3.6, 0.060, 3.9, and 0.32, respectively.

The values of $\widetilde{\Delta t}$ only depend on the diffusion operator, however, so they are unchanged: 0.19 for FS-$D_{TR}R$ and 0.040 for FS-$D_{S2}R$. Fig. 7 shows the relative L_2 error of the various methods for this problem. The plot of the error is identical to that of the previous problem. However, Condition (10) is much less restrictive. The spectral decay condition (12) is unchanged though. As argued earlier, for methods lacking L-stability the condition $\Delta t \leqslant \widetilde{\Delta t}$ appears to put the operator splitting method in its regime of asymptotic convergence.

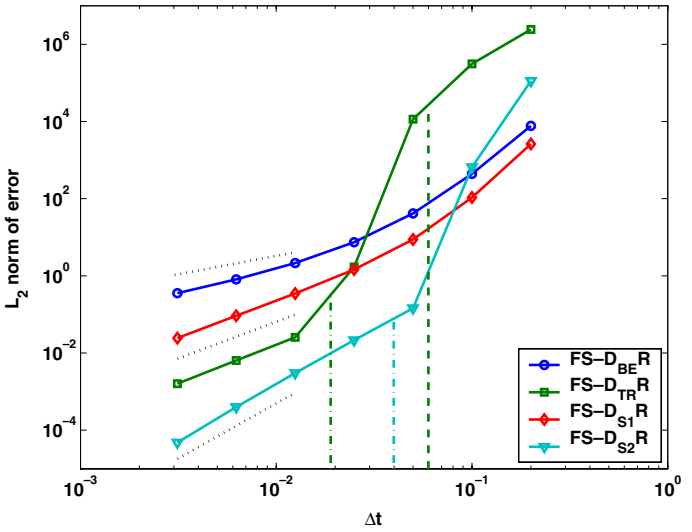

Fig. 7. $\alpha = 1$. L_2 error of the solution of Eq. (14). The dashed lines indicate the values of Δt^* while the dash-dot lines indicate values of $\widetilde{\Delta t}$. FS-D$_{TR}$R is the only method for which the value of Δt^* is within the domain of this graph. The dotted lines are references with first-, second-, and third-order slopes.

7. Stability of operator-splitting methods: C-stability

While A-stability is useful for systems with damping, it is not reasonable nor desirable for systems with growth. Thus, we introduce an extension of A-stability known as C-stability. A method applied to Eq. (5) is C-stable if real numbers Δt^* and C exist such that $|\mathscr{R}(\lambda\Delta t)| \leqslant 1 + C\Delta t$ for $0 < \Delta t \leqslant \Delta t^*$. This type of stability will ensure convergence of the numerical solution at a finite time t as $\Delta t \to 0$. See [2] for more discussion.

For problems of the form of Eq. (5) it is not difficult to show C-stability for many methods. For backward Euler and trapezoidal rule, since they are both A-stable, if $\lambda \leqslant 0$ we can set $\Delta t^* = \infty$ and $C = 0$. If $\lambda > 0$, then for backward Euler we choose $\Delta t^* < \lambda$ and set $C = \lambda/(1 - \lambda\Delta t^*)$. Similarly for trapezoidal we choose $\Delta t^* < 2/\lambda$ and set $C = \lambda/(1 - \lambda\Delta t^*/2)$.

Again, the benefit of C-stability is that it can be applied to problems in which the solution grows rather than decays. Thus, we consider Eq. (6) with $A_R + A_D$ indefinite. We still assume that A_D is a negative definite approximation of the diffusion operator with real negative eigenvalues λ_i as before, but we allow the eigenvalues of A_R to be large enough that the combined system may have positive eigenvalues. If we apply the FS-DR method to this system, then the corresponding C-stability condition is

$$\|\mathscr{R}_{\mathrm{FS-DR}}(\Delta t A_D, \Delta t A_R)\| \leqslant 1 + C\Delta t, \quad 0 < \Delta t < \Delta t^*. \tag{15}$$

We can then develop a theorem similar to Theorem 1.

Theorem 2. *Let Eq. (7) be a time-discretization of Eq. (6). Assume that*

- *A_D is normal with real negative eigenvalues, with $\lambda_n \leqslant \cdots \leqslant \lambda_1 < 0$;*

Let $v_R(\Delta t) = \|\mathscr{R}(\Delta t A_R)\|_{L_2}$. If the following condition holds:

$$\max_i |\mathscr{R}_D(\Delta t\lambda_i)| \leqslant (1 + C\Delta t)/v_R(\Delta t) \quad \text{for } 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty, \tag{16}$$

then the operator splitting method given by Eq. (7) is C-stable, in the sense that Condition (15) is satisfied.

The proof of this theorem is identical to that of Theorem 1, multiplying the right side of the inequalities by $1 + C\Delta t$. Similarly, the following corollary parallels Corollary 1.

Corollary 2. *If $\mathscr{R}_D$ is monotonically increasing on $(-\infty, 0)$, then Condition (16) can be replaced by*

$$\max(|\mathscr{R}_D(\Delta t\lambda_1)|, |\mathscr{R}_D(\Delta t\lambda_n)|) \leqslant (1 + C\Delta t)/v_R(\Delta t) \quad \text{for } 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty. \tag{17}$$

If $\mathscr{R}_D$ is also L-stable, then only Condition (17) simplifies to

$$|\mathscr{R}_D(\Delta t\lambda_1)| \leqslant (1 + C\Delta t)/v_R(\Delta t) \quad \text{for } 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty. \tag{18}$$

In this case where the solution grows, the spectral decay condition (12) is very helpful. Without it, unphysical high wave number modes can grow faster than the physical low wave number modes and pollute the solution.

One drawback with using C-stability as a time step control is that there is often no clear choice for C. A reasonable choice could be a norm of the Jacobian of the right side of the original equation, so in the case of Eq. (6), $C = \|A_D + A_R\|$, for a suitable choice of norm. However, even in the case of a scalar problem using backward Euler for diffusion and an exact solution for the reaction, no value of Δt will satisfy the C-stability condition with this choice of C. Thus, consideration of both the problem and the numerical method is required for a suitable choice of C. As with negative definite systems the stability of indefinite systems also requires bounds on the high and low wave number amplification factors. In addition the spectral decay condition can be applied in this context as well.

8. The Brusselator problem revisited

Here, we revisit the Brusselator problem, using the new stability results of the last section. In the numerical experiments, the Strang RDR split method is implemented, with the SDIRK methods applied to the diffusion step. Since the right side of this system is not a negative definite operator, Corollary 2 applies. We expect the solution to be stable to high frequency perturbations either if the solver for the diffusion step is L-stable or if the time step is sufficiently small.

SDIRK methods are a one-parameter family of methods for solving the equation $u_t = f(t,u)$ by advancing from u^n to u^{n+1} with a time step of Δt by

$$\begin{aligned} k_1 &= f(t + \gamma\Delta t, u^n + \gamma\Delta t k_1),\\ k_2 &= f(t + (1-\gamma)\Delta t, u^n + (1-2\gamma)\Delta t k_1 + \gamma\Delta t k_2),\\ u^{n+1} &= u^n + \frac{\Delta t}{2}(k_1 + k_2). \end{aligned}$$

To avoid a negative time step we choose $\gamma \geqslant 0$. See, e.g., [4].

These methods are at least second-order accurate for all values of γ, but the behavior of the amplification factor varies considerably. For these methods the amplification factor is

$$\mathscr{R}_{SDIRK} = [I - \gamma\Delta t A]^{-2}\left[I + (1-2\gamma)\Delta t A + (\gamma^2 - 2\gamma + 1/2)\Delta t^2 A^2\right].$$

Analysis of the amplification factor shows that these methods will be A-stable if $\gamma > 1/4$, and that $\mathscr{R}(z;\gamma)$ is monotonically increasing for $z \leqslant 0$ if $\gamma > 1/3$. A popular choice of γ is $\frac{3+\sqrt{3}}{6}$, since the method then becomes third order. While the method is A-stable for this value of γ, it is not L-stable, and in fact the amplification factor tends to $-\frac{6(1+\sqrt{3})}{(3+\sqrt{3})^2} \approx -0.7321$ for large Δt. For $\gamma = 1 \pm \frac{1}{\sqrt{2}}$, the method is L-stable; additionally, for

$\gamma = 1 + \frac{1}{\sqrt{2}}$ the amplification factor is monotonically increasing. In addition to these values of γ we also consider $\gamma = 1/2$, for which the amplification factor tends to -1 for large Δt. For this value the method is equivalent to the midpoint rule to leading order.

In Fig. 8, we plot the solution at $t = 32$ with $\Delta t = 1.6 = 0.13\tau$ with three different values of γ: $1 + \frac{1}{\sqrt{2}}$, $\frac{3+\sqrt{3}}{6}$, and 1/2. For $\gamma = 1 + 1/\sqrt{2}$ the solution is smooth and well behaved, while for $\gamma = \frac{3+\sqrt{3}}{6}$ the solution has developed some spatial oscillations. For $\gamma = 1/2$ the solution has developed very jagged spatial oscillations and is clearly unacceptable.

In Fig. 9, we plot the temporal convergence at $t = 80 = 6.7\tau$ for Strang splitting using SDIRK for diffusion with the three different values for γ. For $\gamma = 1 + \frac{1}{\sqrt{2}}$ the convergence is good for all values of Δt. For $\gamma = \frac{3+\sqrt{3}}{6}$ convergence is stalled only for the largest two values of the time step, and we have second order convergence for $\Delta t \leqslant 0.8 = 0.067\tau$. For $\gamma = 0.5$, however, the convergence is poor for a wide range of Δt, and the requirement for second-order convergence is $\Delta t \leqslant 0.0125 \approx 1 \times 10^{-3}\tau$. Note that, because the operators in the Brusselator problem do not commute, using the third-order SDIRK method does not result in third-order convergence for the Strang RDR method for small values of Δt. It does, however, improve the accuracy of the solution, since the error due to the diffusion component is no longer at leading order.

As predicted by Corollary 2, when the diffusion operator is solved with an L-stable method, the method is stable to high wave number instabilities. If the method for diffusion is not L-stable, then a time step restriction is required.

In [15], the instability is also controlled by using an L-stable integrator for the diffusion, though no analysis is presented. Also, the integrator used for the diffusion step, a combination of trapezoidal rule and BDF-2, is not monotonic. Thus, by the theory presented here, the SDIRK method with $\gamma = 1 + 1/\sqrt{2}$ holds some advantage as a method for the diffusion step.

Next, we consider the effect of the spectral decay condition (12) on the Brusselator problem using FS-DR. This condition prevents high wave number modes from dominating low wave number modes. Applying this condition with trapezoidal rule for the diffusion step to get a time step condition gives

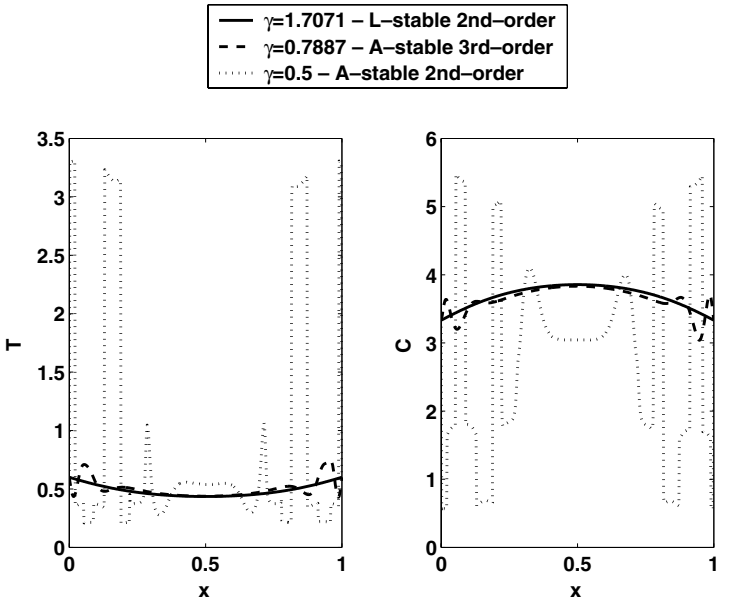

Fig. 8. Solution at $t = 32 \approx 2.7\tau$ ($\Delta t = 1.6 \approx 0.17\tau$) using SDIRK for the diffusion term with $\gamma = 1 + \frac{1}{\sqrt{2}}$, $\gamma = \frac{3+\sqrt{3}}{6}$, and $\gamma = 1/2$ ($\tau = 12$).

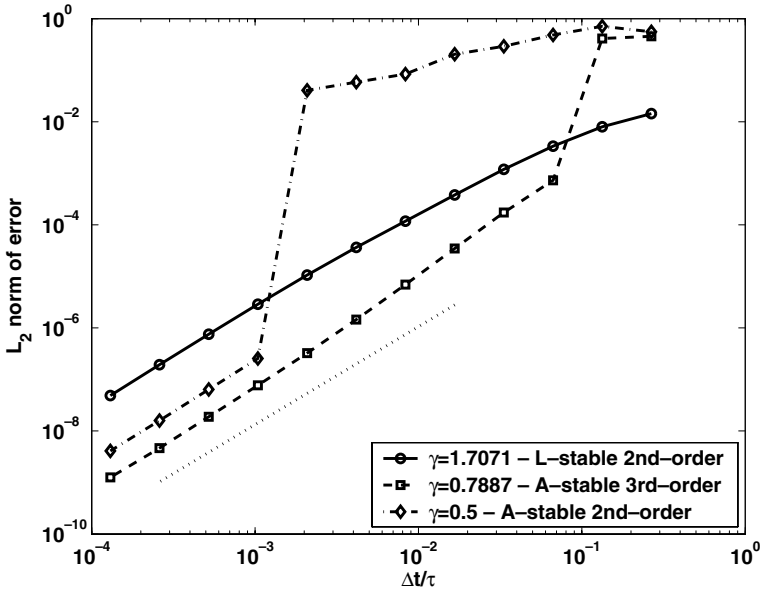

Fig. 9. Temporal convergence at $t = 80 \approx 6.7\tau$ using SDIRK methods for the diffusion term ($\tau = 12$). The dotted line is a reference with second-order slope.

$$\left|\frac{1+\frac{1}{2}\lambda_n\Delta t}{1-\frac{1}{2}\lambda_n\Delta t}\right| \leqslant \left|\frac{1+\frac{1}{2}\lambda_1\Delta t}{1-\frac{1}{2}\lambda_1\Delta t}\right|.$$

We assume that the amplification factor is negative for $\Delta t\lambda_n$ and positive for $\Delta t\lambda_1$ and arrive at the condition

$$\Delta t \leqslant \frac{2}{\sqrt{\lambda_1\lambda_n}}.$$

Because the solution has Dirichlet boundary conditions and has a domain of unit length, λ_1 is closely approximated by $\min(D_1,D_2)\pi^2 \approx 0.2467$. Because the spatial discretization uses linear finite elements, λ_n is closely approximated by $\max(D_1,D_2)(12/\Delta x^2) = 0.3/\Delta x^2$. Thus, the time step condition is

$$\Delta t \leqslant \widetilde{\Delta t} = \frac{\Delta x}{\pi\sqrt{3\max_i D_i \min_i D_i}} \approx 7.351\Delta x. \tag{19}$$

We check this for Strang RDR using grid spacings of $\Delta x = 0.008$, 0.004, 0.002, 0.001, and 0.0005.

Figs. 10 and 11 show the temporal convergence of Strang RDR and Strang DRD for these values of Δx. There is very good agreement with the computed values of $\widetilde{\Delta t}$ and the values of Δt below which these methods are convergent. The values of $\widetilde{\Delta t}$ shift to the right in the Fig. 11 because Strang DRD has two half-steps of the diffusion solve per time step rather than one full-step as in Strang RDR.

9. Conclusion

In this paper, we have presented an analysis of the stability of operator-splitting methods for systems with indefinite operators, including negative definite systems with an indefinite component operator and

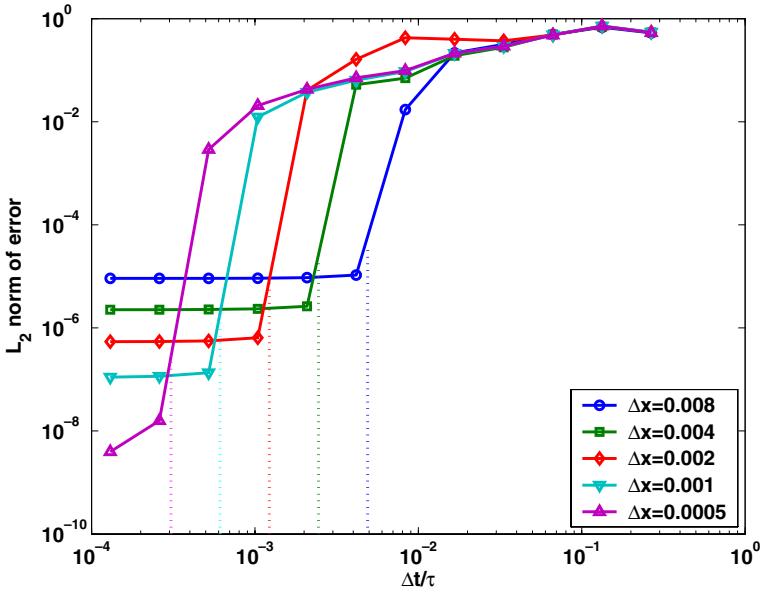

Fig. 10. Brusselator temporal convergence of Strang RDR at $t = 80 \approx 6.7\tau$ for various values of Δx. Dotted lines indicate values of $\widetilde{\Delta t}/\tau$ computed using Eq. (19) ($\tau = 12$).

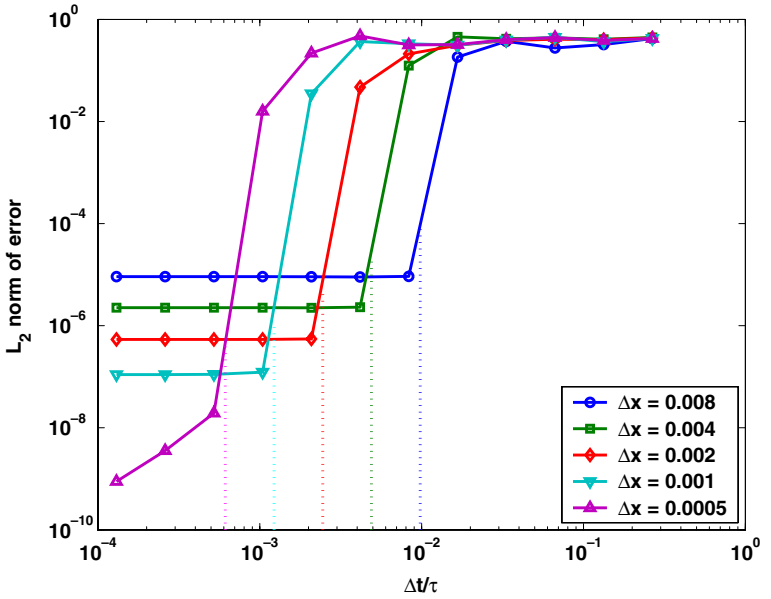

Fig. 11. Brusselator temporal convergence of Strang DRD at $t = 80 \approx 6.7\tau$ for various values of Δx. Dotted lines indicate values of $\widetilde{\Delta t}/\tau$ computed using Eq. (19) ($\tau = 12$).

indefinite systems. The results of this analysis have demonstrated the importance of the spectral decay properties of the amplification factors for the integration of the diffusion operator.

These results were used to explore the convergence problems experienced by some operator split methods when solving the Brusselator problem. We have shown experimentally that if the method used for the

diffusion step is not L-stable, such as trapezoidal rule or certain SDIRK methods, the time step will have an upper bound above which the convergence will be poor. This observation is confirmed by the stability analysis which proved that for a linear problem, if the method for the diffusion step is not L-stable and the time step exceeds some limit, then high wave number modes will pollute the solution.

This analysis also demonstrated that a time step condition may be required even if the method for the diffusion step is L-stable, but in this case the transition from poor, or no convergence to good convergence is not as dramatic because here it is low wave number modes which pollute the solution. However, in contrast to the high wave number instability, which is very clearly identifiable, this low wave number instability is more subtle. These low wave number modes could appear to be physically realistic and not easily identified as instabilities.

Finally, the use of the trapezoidal rule is popular within operator split methods; however, this work demonstrates that it should be used with caution or the convergence may behave disastrously. Future work will develop a time step control procedure based on the observations here so that methods which are not L-stable may be safely used within operator split methods.

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