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

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ABSTRACT

This brief paper presents an A-stability result for operator splitting type time integration methods applied to advection–diffusion–reaction equations with possibly indefinite source terms. These results extend our earlier work on diffusion–reaction systems [D.L. Ropp, J.N. Shadid, Stability of operator splitting methods for systems with indefinite operators: reaction–diffusion systems, J. Comput. Phys. 203 (2) (2005) 449–466]. The A-stability result presents sufficient conditions that control 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. Numerical results are presented that verify second-order convergence for the operator splitting methods and demonstrate control of instabilities on a chemotaxis problem by use of an L-stable diffusion integrator.

1. Introduction

An earlier paper [12] studied the stability of operator splitting methods applied to diffusion–reaction systems. For such systems, if the reaction term is positive definite or semi-definite, instabilities may arise in the numerical solution. A very dramatic example of this is given with the Brusselator problem, using a common second-order Strang splitting method. In this study the reaction term was integrated with a higher order method (CVODE [2]) and the A-stable trapezoidal rule (TR) was used for the diffusion term. The results of this study demonstrated that the Strang operator splitting method produced spurious high wave number oscillations in the solution for larger time steps in contrast to fully-implicit time integration. Intuitively, the splitting of the stabilizing diffusion operator from the indefinite reaction operator, allowed the reaction sub-step to effectively introduce high frequency spurious modes into the solution that would not be instantaneously smoothed by the decoupled diffusion operator. Because the trapezoidal rule has only very weak damping of high wave numbers, these modes could grow during the reaction step and would not be sufficiently damped in the diffusion step.

These observations were developed into an A-stability theory specifying the time step restrictions for such systems. The result in [12] shows that if the amplification factor for the diffusion sub-step, $\mathcal{R}_D$, is monotonically increasing on $(-\infty, 0)$, which is the case for many A-stable methods such as backward Euler and trapezoidal rule, then there exists a time step restriction on the magnitude of the amplification factor for both the smallest and largest wave numbers. If an L-stable meth-

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od is used for the diffusion step, however, the time step condition for high wave number modes can essentially be avoided because these modes will be properly damped. Interestingly, a time step restriction for low wave number modes may still be required when L-stable methods are used, but typically this condition is not as restrictive (see [12] for more details). In this brief paper we extend this type of analysis to advection–diffusion–reaction equations developing an A-stability result and presenting two numerical experiments that demonstrate the theory.

2. Operator splitting and advection–diffusion–reaction systems

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 [17]. 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 a set of single term equations. The most common second-order operator splitting methods of this type are those of Strang [15] and Marchuk [9]. 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

$$\frac{du}{dt} = F_A(u) + F_D(u) + F_R(u), \quad x \in \Omega, \quad t > 0, \tag{1a}$$

$$u = 0, \quad x \in \partial\Omega, \quad t > 0. \tag{1b}$$

In the above, u is the solution vector and $F_A(u)$, $F_D(u)$ and $F_R(u)$ are the advection, diffusion and reaction terms. We then split the terms, creating three 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

$$\frac{du^*}{dt} = F_A(u^*) \quad \text{on } (t^n, t^{n+1}), \quad u^*(t^n) = u^n, \tag{2a}$$

$$\frac{du^{**}}{dt} = F_D(u^{**}) \quad \text{on } (t^n, t^{n+1}), \quad u^{**}(t^n) = u^*(t^{n+1}), \tag{2b}$$

$$\frac{du^{***}}{dt} = F_R(u^{***}) \quad \text{on } (t^n, t^{n+1}), \quad u^{***}(t^n) = u^{**}(t^{n+1}), \tag{2c}$$

with $u^{n+1} = u^{***}(t^{n+1})$. Note that step (2c) has no spatial dependence and thus is essentially an ordinary differential equation (ODE) at each node, requiring no boundary conditions. Steps (2a and 2b) do have spatial dependence, however and thus require application of appropriate boundary conditions.

Using operator notation we denote the solution of a step as $u^* = S_{\alpha,\Delta t}u^n$, where $\alpha = A$, D, or R to denote the different substep solution operators. Thus, the above method can be written as $u^{n+1} = S_{R,\Delta t}S_{D,\Delta t}S_{A,\Delta t}u^n$. We will refer to this method as First-order Splitting – Advection Diffusion Reaction, or FS-RDA. Note that the abbreviation we use orders the operators as they appear in the method; i.e., a step of FS-RDA first applies the advection step, then the diffusion step and finally the reaction step. We can reorder the operators and in some situations this may improve the accuracy of the method; see [14].

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 $u^{n+1} = S_{A,\Delta t/2}S_{D,\Delta t/2}S_{R,\Delta t}S_{D,\Delta t/2}S_{A,\Delta t/2}u^n$. Known as Strang or Marchuk splitting, we shall refer to it as Strang-ADRDA.

Within a step of either FS-RDA or Strang-ADRDA, we can choose how to integrate the advection, diffusion and reaction 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 [2], which implements variable-order (up to fifth-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-RDA or Strang-ADRDA we allow CVODE to take several smaller steps to insure that this step produces a very accurate solution.

In our numerical computations we employ a finite element discretization of the advection–diffusion–reaction system (1). The advection and diffusion steps are solved globally by implicit methods. The diffusion step is integrated using a single step of a one-step method, such as backward Euler or trapezoidal rule, or by a multi-stage method such as SDIRK [1]. For the advection step we enforce additional constraints to preserve positivity and monotonicity. For this we use the implicit FEM-FCT method (see [7]), an implementation of flux-corrected transport for finite elements schemes based on the θ-method. This results in a system identical to Eq. (2) but with the u, F_R, F_D and F_A replaced by their discretized representations. The discretized representations of F_A and F_D incorporate contributions from the mass matrix of the transient term.

3. Stability of operator splitting methods: A-stability

The definitions of stability we use here consider the linear system

$$\frac{du}{dt} = \lambda u, \quad u(0) = u_0, \tag{3}$$

where λ is a complex constant. For an advection–diffusion–reaction system, the diffusion and reaction terms typically correspond to the real components of λ while the advection term corresponds to the imaginary component. After temporal discretization using a one-step method, this equation becomes a difference equation of the form

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

Here $\mathcal{R}(\Delta t\lambda)$, called the amplification factor or stability matrix, 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

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

The method is considered absolutely stable, or A-stable, at a value $z \in \mathbb{C}$ if $|\mathcal{R}(z)| \leqslant 1$. 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 $|\mathcal{R}(z)| \leqslant 1$ 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, which adds to A-stability the condition that $\lim_{z\to-\infty}\mathcal{R}(z) = 0$. This ensures that the $\mathcal{R}$ 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 $\lim_{z\to-\infty}\mathcal{R}(z) = -1$ for trapezoidal rule and unphysical high wave number modes decay slowly.

We study the stability of a split system such as Eq. (2) similarly. We assume Eq. (1) represents a system that has been spatially discretized and that all the terms are linear with constant coefficients, with $F_\alpha(u) = A_\alpha u,\ \alpha = A, D, R$. Then Eq. (1) is written as

$$\frac{du}{dt} = A_A u + A_D u + A_R u, \quad x \in \Omega, \quad t > 0, \tag{4a}$$
$$u = 0, \quad x \in \partial\Omega, \quad t > 0. \tag{4b}$$

where $u \in \mathbb{R}^N$ and $A_A, A_D, A_R \in \mathbb{R}^{N\times N}$. Using FS-ADR with solution methods $S_{A,\Delta t} = \mathcal{R}_A(\Delta t A_A), S_{D,\Delta t} = \mathcal{R}_D(\Delta t A_D)$, and $S_{R,\Delta t} = \mathcal{R}_R(\Delta t A_R)$, our discretized system is

$$\begin{aligned} u^* &= \mathcal{R}_R(\Delta t A_R)u^n, \\ u^{**} &= \mathcal{R}_D(\Delta t A_D)u^*, \\ u^{n+1} &= \mathcal{R}_A(\Delta t A_A)u^{**}, \end{aligned} \tag{5}$$

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

$$u^{n+1} = \mathcal{R}_A(\Delta t A_A)\mathcal{R}_D(\Delta t A_D)\mathcal{R}_R(\Delta t A_R)u^n,$$

or

$$u^{n+1} = \mathcal{R}_{\text{FS-ADR}}(\Delta t A_A, \Delta t A_D, \Delta t A_R)u^n,$$

where $\mathcal{R}_{\text{FS-ADR}}(\Delta t A_A, \Delta t A_D, \Delta t A_R) = \mathcal{R}_A(\Delta t A_A)\mathcal{R}_D(\Delta t A_D)\mathcal{R}_R(\Delta t A_R)$. The condition for A-stability is similar to that for the scalar ODE above:

$$\|\mathcal{R}_{\text{FS-ADR}}(\Delta t A_A, \Delta t A_D, \Delta t A_R)\| \leqslant 1, \quad 0 < \Delta t \leqslant \Delta t^*. \tag{6}$$

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. Stability results of split schemes when all the terms are negative definite can be found in [3,4].

We are interested initially in A-stability for FS-ADR, so we assume that $A_A + A_D + A_R$ is negative definite. If we neglect boundary conditions, we can assume that the A_α are normal matrices with a complete set of eigenvalues $\lambda_{\alpha,i}$. In that case, for a rational polynomial $p(z)$, we have

$$\|p(\mathcal{R}_\alpha(\Delta t A_\alpha))\| = \max_i |p(\Delta t\lambda_{\alpha,i})|.$$

The discrete diffusion matrix A_D will typically be negative definite with real negative eigenvalues $\lambda_{D,N} \leqslant \cdots \leqslant \lambda_{D,1} \leqslant 0$. The discrete advection matrix A_A has eigenvalues with imaginary components. Typically if A_A arises from central difference approximations, the eigenvalues $\lambda_{A,i}$ will be purely imaginary, while if it arises from an upwinding the $\lambda_{A,i}$ may have real components as well. We do not make any assumption about the reaction term, however, except that $A_D + A_R + A_A$ is negative definite. Thus, A_R may have eigenvalues with positive real part, so that the solution grows during the reaction step.

We assume that both the diffusion and the advection steps are solved with methods which are A-stable, that is, $\|\mathcal{R}_\alpha(\Delta t A_\alpha)\| \leqslant 1$ for $\alpha = A, D$. For the advection step, ideally there is no growth or damping, so it is best if this norm stays very close to 1. Even if the method for advection is not unconditionally stable, we expect that the time step is chosen small enough so that the method is stable.

In practice the reaction step can be solved locally at each node, so it is solved with an ODE integrator that is subcycled with very strict accuracy tolerances, so it is reasonable to assume the step is solved exactly. Naturally, the accuracy of this step is limited to the accuracy of the reaction step solved in isolation and will not capture any interactions with the advection and diffusion terms. The advection and diffusion steps depend on global information, however, so these are typically solved with one-step of a single step method, such as backward Euler, trapezoidal rule, or (more generally) Runge–Kutta methods. The following theorem shows the time step restrictions required for the FS-ADR method to be A-stable.

Theorem 1. *Let Eq. (5) be an operator split time-discretization of Eq. (4). Assume that*

- $A_A + A_D + A_R$ *is negative definite;*
- A_D *is normal with real negative eigenvalues, with* $\lambda_n \leqslant \cdots \leqslant \lambda_1 < 0$*;*
- $\|\mathcal{R}_A(\Delta t A_A)\|_{L_2} \leqslant 1$ *for* $\Delta t \leqslant \Delta t_A \leqslant \infty$.

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

$$\max_i |\mathcal{R}_D(\Delta t \lambda_i)| \leqslant 1/v_R(\Delta t) \quad \text{for} \quad 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty, \tag{7}$$

then the operator splitting method given by Eq. (5) is stable for $\Delta t \leqslant \min(\Delta t_A, \Delta t^*)$, *in the sense that Condition (6) is satisfied.*

Proof.

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

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

Using Condition (7) with this relation guarantees

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

Because $\mathcal{R}_A$ is A-stable, this gives

$$\|\mathcal{R}_{\text{FS-ADR}}(\Delta t A_D, \Delta t A_R)\|_{L_2} \leqslant \|\mathcal{R}_A(\Delta t A_A)\|_{L_2} \|\mathcal{R}_D(\Delta t A_D)\|_{L_2} \|\mathcal{R}_R(\Delta t A_R)\|_{L_2} \leqslant 1.$$

Hence, this splitting method is A-stable. □

As we noted before, ideally $\|\mathcal{R}_A(\Delta t A_A)\|$ is close to 1. Thus, we formulated the above condition as a restriction on $\mathcal{R}_D(\Delta t A_D)$, so as not to require damping in the advection step. If no physical dissipation is present then the stability of the method will be controlled by the dissipation introduced by the advection method. We do not consider this case in the present study.

With the above conditions this is essentially the same restriction that was required for reaction–diffusion systems. In that case, it was found that the situation simplifies if $\mathcal{R}_D$ 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 $\mathcal{R}_D$ is L-stable. We state the result from [12] in the case of these simplifications.

Corollary 1. *If* $\mathcal{R}_D$ *is monotonically increasing on* $(-\infty, 0)$, *then Condition (7) can be replaced by*

$$\max(|\mathcal{R}_D(\Delta t \lambda_1)|, |\mathcal{R}_D(\Delta t \lambda_n)|) \leqslant 1/v_R(\Delta t) \quad \text{for} \quad 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty. \tag{8}$$

If $\mathcal{R}_D$ *is also L-stable, then Condition (8) simplifies to*

$$|\mathcal{R}_D(\Delta t \lambda_1)| \leqslant 1/v_R(\Delta t) \quad \text{for} \quad 0 \leqslant \Delta t \leqslant \Delta t^* \leqslant \infty. \tag{9}$$

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

$$\mathcal{R}_{\text{Strang ARDRA}} = \mathcal{R}_A\left(\frac{\Delta t}{2} A_A\right) \mathcal{R}_R\left(\frac{\Delta t}{2} A_R\right) \mathcal{R}_D(\Delta t A_D) \mathcal{R}_R\left(\frac{\Delta t}{2} A_R\right) \mathcal{R}_A\left(\frac{\Delta t}{2} A_A\right).$$

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

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.

4. Test cases

4.1. Thermal Wave

The first test problem that we will describe is associated with the solution to the time-dependent heat equation with advection, diffusion and a nonlinear source term. This is a generalization of the diffusion–reaction test problem of Knio et al. [5] and provides a numerical example with a smooth analytic solution in the form of a propagating wave. The nonlinear advection–diffusion–reaction equation is

$$\frac{\partial T}{\partial t} = \nu \frac{\partial^2 T}{\partial x^2} + \frac{\epsilon}{\delta}\frac{\partial T}{\partial x} + \frac{8\nu}{\delta^2} T^2 (1 - T), \tag{10}$$

where the boundary conditions are $T(x = -\infty, t) = 1$ and $T(x = \infty, t) = 0$. The parameter, $\delta > 0$, can be freely selected but does not change the ratio of time scales between the diffusion and the reaction terms. The analytic solution is

$$T(x,t) = \frac{1}{2}\left(1 - \tanh\left[\frac{x - (2\nu - \epsilon)t/\delta}{\delta}\right]\right). \tag{11}$$

In our example we select $\delta = \epsilon = \nu = 1$ and solve this equation on the domain $-10 \leqslant x \leqslant 10$. The simulation was integrated to $t_{final} = 2.048$ with a mesh spacing of $\Delta x = 0.04$. Since the solution is a wave front with a speed of $c = 1$, we use the CFL condition to define a characteristic time scale of $\tau = \Delta x/c = 0.04$. The results for the first and second-order splittings are presented in Figs. 1 and 2 for a mesh with $\Delta x = 0.04$ and in Fig. 3 for Strang splitting on a finer mesh with $\Delta x = 0.005$. The error that we report here is the ratio of the L_2 norm of the difference of the numerical solution and the exact solution. Here we see that after a pre-asymptotic region the expected first- and second-order convergence is achieved for this negative definite problem with the A-stable backward Euler and trapezoidal rule integrators. Figs. 1 and 2 show that at sufficiently small time steps the spatial error, in a subset of the first-order splittings and all the Strang splitting methods, begins to dominate and the error norm begins to plateau at this value.

Comparing Figs. 2 and 3 for the Strang splitting method the decrease in the magnitude of the plateau in the error for small time steps is evident. The order-of-accuracy for the spatial discretization is roughly estimated from these two error plateaus as 1.98 which is very close to the expected second-order convergence for a Galerkin FE type method using linear interpolation for smooth solutions [10].

4.2. Chemotaxis model

The second test problem is a simplified model of chemotaxis that was first proposed by Tyson et al. [16]. Mathematical models of chemotaxis are applied to study pattern formation in biological organisms that exhibit a biased random walk in

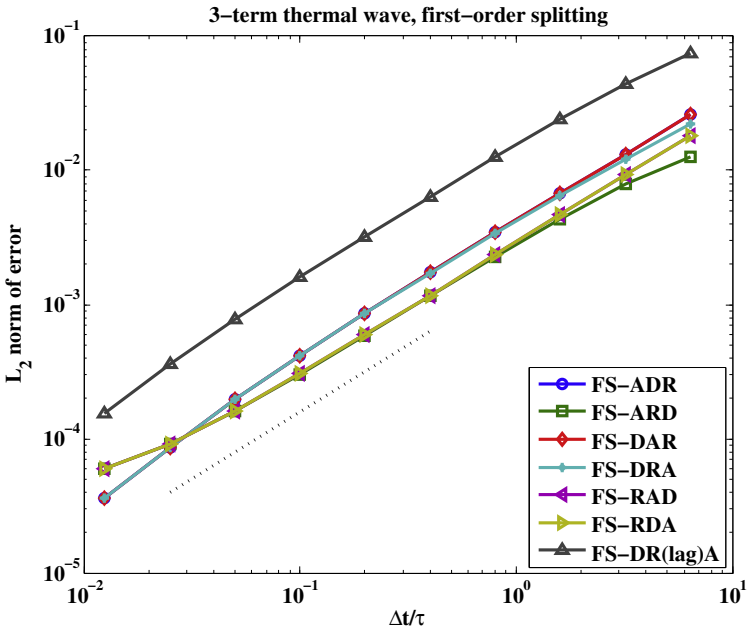

Fig. 1. Temporal convergence of the first-order splitting methods on the Thermal Wave problem on the $\Delta x = 0.04$ mesh. The FS-DR(lag)A case uses a source term which is explicit (or lagged) and based on the last time step solution. The dotted line is a reference with first-order slope.

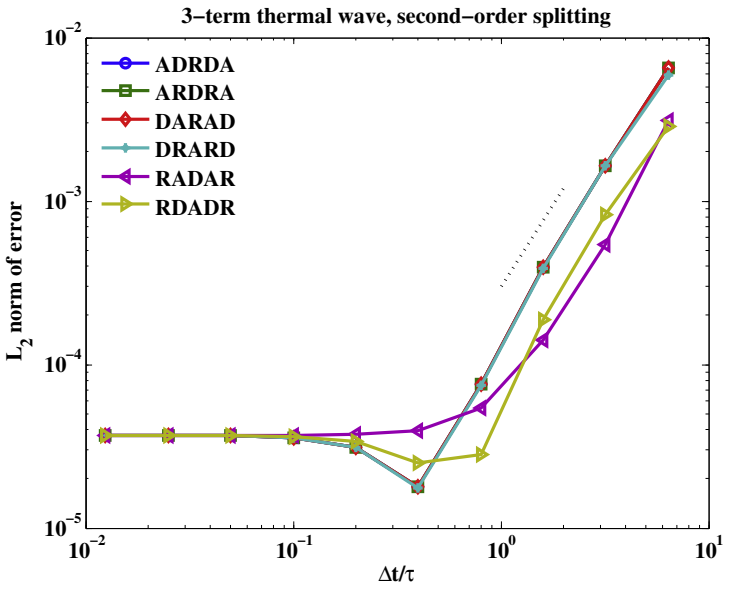

Fig. 2. Temporal convergence of second-order Strang splitting methods with different ordering of operators, using the trapezoidal rule for the advection step on the $\Delta x = 0.04$ mesh. The dotted line is a reference with second-order slope.

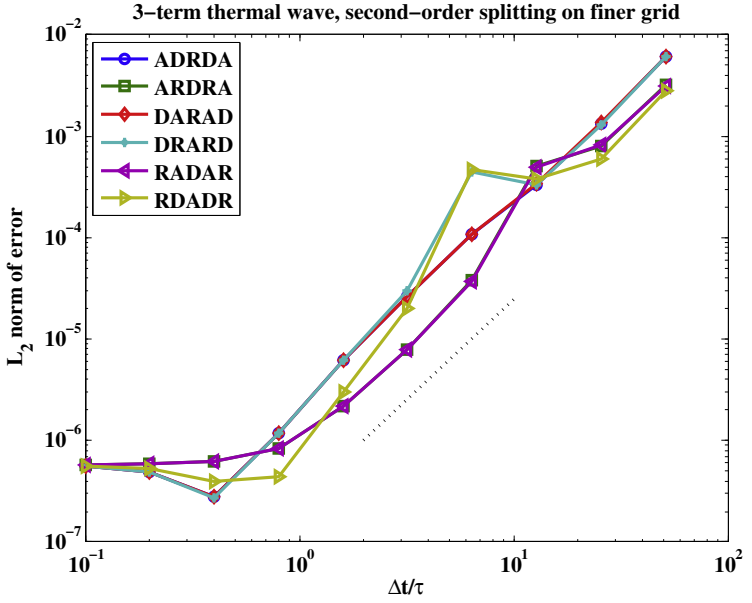

Fig. 3. Temporal convergence of second-order Strang splitting methods with different ordering of operators, using the trapezoidal rule for the advection step on the $\Delta x = 0.005$ mesh. The dotted line is a reference with second-order slope.

the presence of a chemical [16]. These equations model a cell density (n) in the presence of a chemoattractant concentration (c) in which both the cells and the chemoattractant diffuse, while the gradient of the chemical concentration directs the advection of the cells. The equations are

$$\frac{\partial n}{\partial t} + [\alpha \nabla c] \cdot \nabla n - D_n \nabla^2 n + \left(\alpha \nabla^2 c\right) n = 0,$$
$$\frac{\partial c}{\partial t} - D_c \nabla^2 c + nc = 0.$$

We solve this problem on the domain $0 \leqslant x \leqslant 10$ and set $\partial n/\partial x = \partial c/\partial x = 0$ on both boundaries. We also set $D_n = D_c = 0.1$ and $\alpha = 2$ and use initial conditions

$$n(t=0)=1, \quad c(t=0)=1-\frac{\cos(\pi x/5)}{4}.$$

The simulation was integrated to $t=3$ with a mesh spacing of $\Delta x=0.1$. Since there is not a closed form analytical solution for this problem 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 based on a two-point Richardson extrapolation of the solution for each of the operator split methods. This choice allows the spatial discretization error to be eliminated from the error norm calculation for sufficiently refined spatial meshes [10,13,12].

The chemotaxis system is very similar to the Brusselator system which was used to illustrate the destabilizing effects of splitting off the dissipative diffusion operator from reaction in [12,13]. For the chemotaxis model it can be seen that the cell density source term can become indefinite as the concavity of the chemoattractant, c, varies. Fig. 4 shows the solution of the chemotaxis system at three different solution times when an A-stable diffusion integrator is used in a Strang splitting method. At time $t=1$ the incipient growth of high wave number disturbances is apparent. At later times the high wave number modes have saturated and are clearly evident.

To analyze the effect of the introduction of spurious high wave number modes in this problem, we carry out an order-of-accuracy study for a first-order splitting method that uses an A-stable or L-stable integrator for the diffusion step as in [12,13]. The results are presented in Figs. 5 and 6. In these plots the characteristic time scale that is used to normalize the time step sizes is based on the diffusion time scale $\tau=(\Delta x)^2/\max(D_n,D_c)=0.1$. Based roughly on the initial conditions and the evolution of the profiles this is the fastest time scale of the chemotaxis problem. As is clearly seen in Fig. 5 the use of an A-stable integrator produces a very significant degradation of accuracy in the method at large time steps that include the case of $\Delta t=0.5$ as used in the results shown in Fig. 4. This instability, as in the case for the Brusselator, produces high wave number spurious modes which pollute the solution and are not damped by the A-stable trapezoidal rule integrator. While the FCT method used in our advection step does add controlled amounts of dissipation to solve the hyperbolic advection operator, this dissipation is not sufficient to control the oscillations when coupled with an A-stable diffusion integrator such as the TR. Finally it should be noted that this Strang splitting method does not achieve its asymptotic order-of-accuracy until the time step size roughly resolves the fastest component time scale that is on the order of the diffusion time scale. This type of behavior, for a technique that employs implicit sub-step solvers, is very disconcerting and is in stark contrast to fully-implicit type methods using the same A-stable time integration methods (see for example [6,10,13]).

In contrast when the L-stable SDIRK method is used for integrating the diffusion operator, which strongly damps the highest unphysical wave numbers, the splitting method is verified to be stable as shown in Fig. 6. Our numerical results complement the results of [16] which demonstrated similar behavior for an L-stable diffusion integrator. In [16] Tyson, Stern and LeVeque presented a persuasive intuitive argument that the use of an L-stable integrator will help to suppress the unphysical

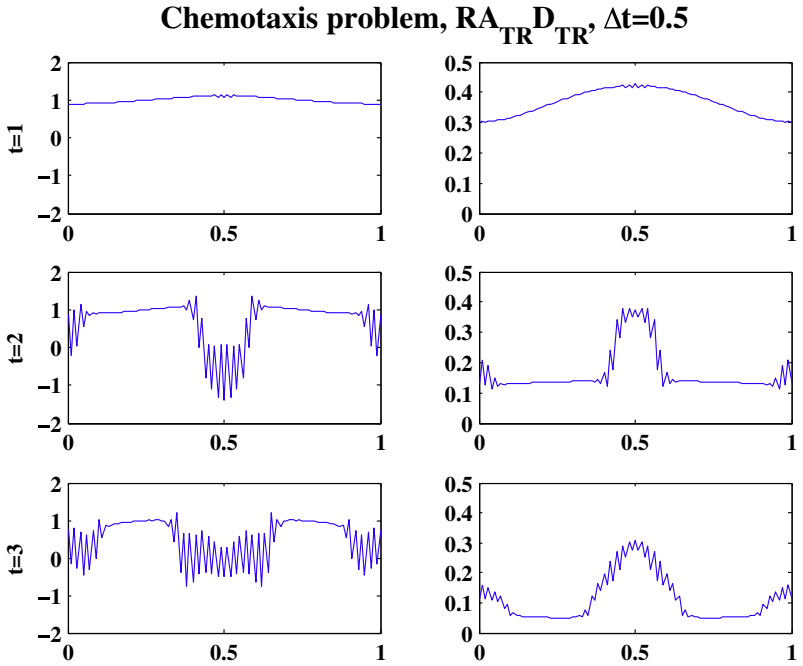

Fig. 4. Solution profiles of the operator split integrator with A-stable TR diffusion integrator. The chemoattractant concentration (c) is on the left and the cell density (n) is on the right. These solutions clearly show incipient growth of high wave number spurious modes ($t=1$) and saturated modes at later times.

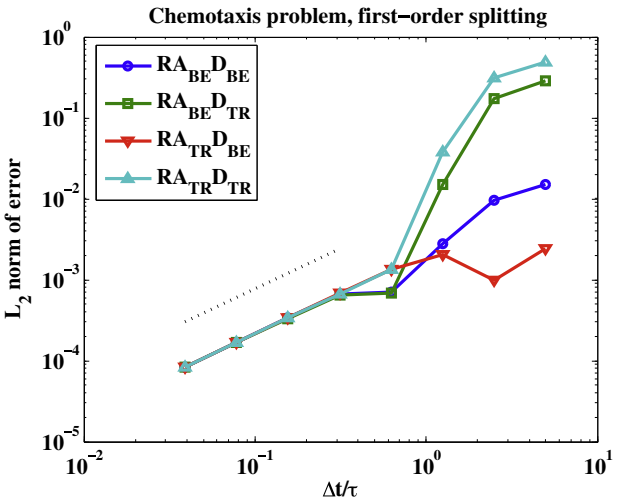

Fig. 5. Temporal convergence of FS-RAD, using either backward Euler or trapezoidal rule for the advection and diffusion steps. The dotted line is a reference with first-order slope.

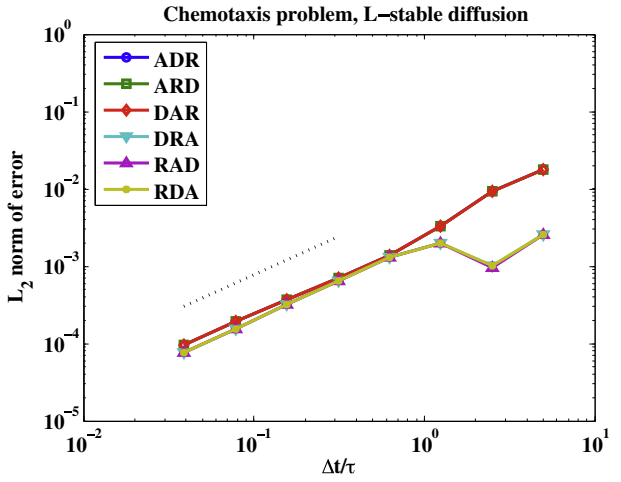

Fig. 6. Temporal convergence of FS with different ordering of operators, using trapezoidal rule for the advection step and the L-stable SDIRK for the diffusion step. The dotted line is a reference with first-order slope. The plots for ADR, ARD and DAR are nearly identical, as are the plots for DRA, RAD and RDA.

high wave number oscillations. That study also numerically demonstrated that the TR-BDF2 method, that is L-stable, successfully controlled these instabilities. In the context of our Theorem 1 the TR-BDF2 method does not have a monotone amplification factor and therefore does not satisfy the conditions for Corollary 1. This makes verifying the sufficient conditions for A-stability of the operator splitting method more difficult. In practice for this problem however, the L-stability property of the diffusion integrator for both TR-BDF2 and SDIRK, effectively damps the unphysical high wave number modes and stabilizes the operator splitting method. These results are consistent with the result of Theorem 1 and help to further explain the results presented in the very illuminating numerical results of [16].

5. Conclusions

In this paper we have presented a new theoretical result and numerical computations for the stability of operator split time integration of advection–diffusion–reaction systems with indefinite operators. This A-stability result has extended our work in [12] for diffusion–reaction 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 systems with indefinite source terms such as the chemotaxis problem. We have shown experimentally that if the method used for the diffusion step is not

L-stable, such as the trapezoidal rule, 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. 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.

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