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A note on iterated splitting schemes

Willem Hundsdorfer[a], Laura Portero[b,*]

[a] *CWI, Kruislaan 413, Amsterdam, The Netherlands*
[b] *Departamento de Matemática e Informática, Universidad Pública de Navarra, Campus de Arrosadía s/n, 31006 Pamplona, Spain*

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Abstract

Iterated splittings seem attractive in view of consistency and local accuracy. In this note it will be shown, however, that for stiff systems the stability properties are quite poor. Specific Runge–Kutta implementations can improve stability, but this leads to classes of methods that are better studied in their own right.

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1. Iterated splitting

In this short note we consider an iterated splitting procedure applied to stiff systems of ordinary differential equations (ODEs) in $\mathbb{R}^M$. The system is written as

$$u'(t) = F(t, u(t)), \quad u(0) = u_0, \tag{1.1}$$

with a time integration interval $[0, T]$. In applications these systems are often obtained by spatial discretizations of initial-boundary value problems for partial differential equations (PDEs); such a semi-discretization leads to stiff systems (1.1) of very large dimension M. Often it is possible to decompose F into two simpler functions

$$F(t, v) = F_1(t, v) + F_2(t, v) \quad \text{for } t \geqslant 0, \quad v \in \mathbb{R}^M. \tag{1.2}$$

Splitting methods are based on such a decomposition. In the following we denote by $\tau > 0$ the step size and $u_n \approx u(t_n)$ stands for the numerical approximation at time level $t_n = n\tau$, $n \geqslant 0$.

We study the following *iterated splitting* scheme: on each time interval $[t_n, t_{n+1}]$ we start with a prediction $v_0(t)$ for the solution and then solve for $i = 1, 2, \ldots, m$ subsequently

$$\bar{v}_i'(t) = F_1(t, \bar{v}_i(t)) + F_2(t, v_{i-1}(t)), \quad \bar{v}_i(t_n) = u_n, \tag{1.3a}$$

$$v_i'(t) = F_1(t, \bar{v}_i(t)) + F_2(t, v_i(t)), \quad v_i(t_n) = u_n, \tag{1.3b}$$

* Corresponding author. Tel.: +34 948168055; fax: +34 948169521.
E-mail address: laura.portero@unavarra.es (L. Portero).

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giving the approximation $u_{n+1} = v_m(t_{n+1})$ at the new time level t_{n+1}. In this note we consider fixed, low values of m, in particular $m = 1$ or $m = 2$. Moreover, we shall primarily consider autonomous problems with initial approximation $v_0(t) = u_n$; for non-autonomous problems arising from PDEs with time-dependent boundary conditions the initial approximation should be adapted to match the boundary conditions.

Compared to standard fractional step methods, this approach offers the advantage that all stages remain consistent with the full equation (1.1). If we take one step beginning on the exact solution $u_n = u(t_n)$ and $v_0(t) = u_n$, then it is not too difficult to show that $u(t_{n+1}) - u_{n+1} = \mathcal{O}(\tau^{2m+1})$, that is, consistency of order $2m$. Of course, the steps in (1.3) should also be solved numerically with sufficient high accuracy.

This type of iterated splitting was recently considered by Kanney et al. [6] and by Faragó and Geiser [3]. However, in these papers stability estimates for stiff systems are lacking. The object of this note is to show that the stability properties of (1.3) are quite poor in general. This makes the approach unattractive for stiff systems.

As we shall see, specific discretizations of (1.3) are possible that have better stability properties than the continuous system (1.3) itself, but these lead to splitting methods of the fractional step Runge–Kutta type [1,2] that are better studied in their own right without reference to (1.3).

2. Stability for linear equations

2.1. Recursions

Stability will be studied for linear problems with

$$F_k(t, v) = A_k v, \quad k = 1, 2. \tag{2.1}$$

We consider some suitable vector norm $\|\cdot\|$ on $\mathbb{R}^M$, together with its induced operator norm. The matrix exponential of $Z \in \mathbb{R}^{M\times M}$ will be denoted by e^Z. It will be assumed that

$$\|\mathrm{e}^{\tau A_k}\| \leqslant 1 \quad \text{for all } \tau > 0, \quad k = 1, 2. \tag{2.2}$$

In terms of logarithmic matrix norms, see for example [5], this means that $\mu(A_k) \leqslant 0$. This implies $\mu(A_1 + A_2) \leqslant 0$ and therefore $\|\mathrm{e}^{\tau(A_1+A_2)}\| \leqslant 1$, so the system (1.1) itself will be stable.

For the linear problems (2.1) we can employ the variation of constants formula; elimination of the intermediate functions $\bar{v}_i$ then gives

$$\begin{aligned} v_i(t) = &\left(\mathrm{e}^{(t-t_n)A_2} + \int_{s=t_n}^{t} \mathrm{e}^{(t-s)A_2} A_1 \mathrm{e}^{(s-t_n)A_1}\,\mathrm{d}s\right) u_n \\ &+ \int_{s=t_n}^{t}\int_{s'=t_n}^{s} \mathrm{e}^{(t-s)A_2} A_1 \mathrm{e}^{(s-s')A_1} A_2 v_{i-1}(s')\,\mathrm{d}s'\,\mathrm{d}s. \end{aligned} \tag{2.3}$$

The double integral $\int_{s=t_n}^{t}\int_{s'=t_n}^{s}$ can be evaluated as $\int_{s'=t_n}^{t}\int_{s=s'}^{t}$, because the functions involved are continuous, and this will be used below for the commuting case.

2.2. Commuting operators

The formula (2.3) is not very transparent. If the operators A_1 and A_2 commute with well-conditioned system of eigenvectors, we can consider the eigenvalues λ_k of A_k instead of the operators A_k themselves.

Replacing A_k by λ_k, $k = 1, 2$, it follows from (2.3) after some calculations that

$$v_i(t) = \frac{\lambda_1 \mathrm{e}^{(t-t_n)\lambda_1} - \lambda_2 \mathrm{e}^{(t-t_n)\lambda_2}}{\lambda_1 - \lambda_2}\, u_n + \frac{\lambda_1\lambda_2}{\lambda_1 - \lambda_2}\int_{t_n}^{t} (\mathrm{e}^{(t-s)\lambda_1} - \mathrm{e}^{(t-s)\lambda_2}) v_{i-1}(s)\,\mathrm{d}s. \tag{2.4}$$

Note that this relation is *symmetric* in λ_1 and λ_2. Hence, interchanging the operators A_1 and A_2 does not change the iteration errors in this commuting case.

Denote $z_k = \tau\lambda_k$, $k = 1, 2$. Starting with $v_0(t) = u_n$, we will then obtain

$$v_m(t_{n+1}) = S_m(z_1, z_2)u_n, \tag{2.5}$$

where S_m is the stability function of the scheme with m iterations. Using (2.4) it follows by some calculations that

$$S_1(z_1, z_2) = 1 + \frac{z_1 + z_2}{z_1 - z_2}(\mathrm{e}^{z_1} - \mathrm{e}^{z_2}), \tag{2.6}$$

$$S_2(z_1, z_2) = S_1(z_1, z_2) + \frac{z_1 z_2 (z_1 + z_2)}{(z_1 - z_2)^2}\left(\mathrm{e}^{z_1} + \mathrm{e}^{z_2} - 2\frac{\mathrm{e}^{z_1} - \mathrm{e}^{z_2}}{z_1 - z_2}\right). \tag{2.7}$$

2.2.1. $A(\alpha)$-stability

Let us consider the eigenvalues in a wedge

$$\mathscr{W}_\alpha = \{\zeta \in \mathbb{C} : |\arg(-\zeta)| \leqslant \alpha\},$$

with angle α. Instead of $z \in \mathscr{W}_0$ (the non-positive real line) we shall simply write $z \leqslant 0$. It would be ideal to have $|S_m(z_1, z_2)| \leqslant 1$ whenever $z_1, z_2 \in \mathscr{W}_{\pi/2}$, which would amount to A-stability in both components z_1 and z_2. However, this will not hold with these iterated splitting schemes.

In fact, it appears that $|S_m(z_1, z_2)| \leqslant 1$ if $z_1, z_2 \leqslant 0$, but this linear stability property is lost as soon as one of the z_k is allowed to be in a wedge $\mathscr{W}_\alpha$ with positive angle $\alpha > 0$.

Theorem 2.1. *For both $m = 1, 2$, we have*

$$\max_{z_1 \in \mathscr{W}_\alpha, z_2 \leqslant 0} |S_m(z_1, z_2)| \leqslant 1 \implies \alpha = 0.$$

Proof. Considering a fixed $z_1 = z$ and $z_2 \to -\infty$, we obtain

$$S_1(z, -\infty) = 1 - \mathrm{e}^z, \quad S_2(z, -\infty) = 1 - (1 - z)\mathrm{e}^z.$$

If $z = x + \mathrm{i}y$, it follows that

$$|S_1(z, -\infty)| \leqslant 1 \iff \mathrm{e}^x \leqslant 2\cos y.$$

This cannot hold for arbitrary $z \in \mathscr{W}_\alpha$ if $\alpha > 0$, since the imaginary part of such z can assume any value, and in particular we may have $\cos y < 0$. In the same way the result for S_2 follows. □

3. Discretized forms

To test the behaviour of the iterated splittings, numerical experiments were performed for simple linear reaction–diffusion systems, with both A_1 and A_2 having real non-positive eigenvalues, and the fractional steps were discretized with various Runge–Kutta methods. Even for this case with real eigenvalues, instabilities were often observed, due to the discretizations.

3.1. Example: discretizations with θ-methods

We consider discretizations with θ-methods. To model the application of different methods for (1.3a) and (1.3b), we may take different values of the method parameter θ in the stages. So, consider $m = 1$, and let $\theta_1, \theta_2 \geqslant \frac{1}{2}$. For autonomous problems, assume the two stages in (1.3) are discretized as

$$\begin{aligned} \bar{u}_{n+1} &= u_n + \tau(1 - \theta_1)(F_1(u_n) + F_2(u_n)) + \tau\theta_1(F_1(\bar{u}_{n+1}) + F_2(u_n)), \\ u_{n+1} &= u_n + \tau(1 - \theta_2)(F_1(u_n) + F_2(u_n)) + \tau\theta_2(F_1(\bar{u}_{n+1}) + F_2(u_{n+1})). \end{aligned} \tag{3.1}$$

As noted before, for non-autonomous problems arising from PDEs with time-dependent boundary conditions, the initial guess $v_0(t_{n+1})$ should be adapted to match the boundary conditions. Application to the linear systems (2.1), using the notation $Z_k = \tau A_k$, gives

$$u_{n+1} = (I - \theta_2 Z_2)^{-1}(I - \theta_1 Z_1)^{-1} Z_1 (I + (\theta_2 - \theta_1) Z_1) u_n + (I - \theta_2 Z_2)^{-1}(I + (1 - \theta_2) Z_2) u_n + (I - \theta_2 Z_2)^{-1} \theta_2 Z_1 (I - \theta_1 Z_1)^{-1} Z_2 u_n. \tag{3.2}$$

For any fixed Z_2, and $\theta_1 \neq \theta_2$, the first term on the right-hand side will become *unbounded* if one or more eigenvalues of Z_1 tend to $-\infty$. This means that even for one single step, conditions on the step size need to be imposed to prevent instability.

On the other hand, if we take θ_1 and θ_2 equal, say $\theta_k = \theta$, $k = 1, 2$, then

$$u_{n+1} = (I + (I - \theta Z_2)^{-1}(I - \theta Z_1)^{-1}(Z_1 + Z_2)) u_n. \tag{3.3}$$

In fact, the scheme (3.1) then reduces to the Douglas splitting scheme, which is A-stable for $\theta \geqslant \frac{1}{2}$; see e.g., [5]. It is rather surprising that the stability properties of this discrete version are much better than for (2.6).

Remark 3.1. The most interesting case is $\theta = \frac{1}{2}$, for which the scheme will be of order two. For that scheme stability can also be shown for non-commuting operators. Setting $\widehat{u}_n = (I - \frac{1}{2} Z_2) u_n$, we have

$$\widehat{u}_{n+1} = \left(I - \tfrac{1}{2} Z_1\right)^{-1} \left(I + \tfrac{1}{2} Z_1\right) \left(I + \tfrac{1}{2} Z_2\right) \left(I - \tfrac{1}{2} Z_2\right)^{-1} \widehat{u}_n.$$

Assuming (2.2) with an inner-product norm, it follows that the norms of $(I - \frac{1}{2} Z_k)^{-1}$ and $(I - \frac{1}{2} Z_k)^{-1}(I + \frac{1}{2} Z_k)$ are all bounded by 1. (This is just unconditional stability of the implicit Euler method and trapezoidal rule.) Hence $\|\widehat{u}_{n+1}\| \leqslant \|\widehat{u}_n\|$, and

$$\|u_n\| \leqslant \left\| \left(I - \tfrac{1}{2} Z_2\right) u_0 \right\| \quad \text{for all } n \geqslant 0.$$

This gives a stability result provided that $\|Z_2 u_0\| \leqslant C \|u_0\|$. We note that in PDE applications, if A_2 is a discretized spatial derivative operator, then $A_2 u_0$ will be bounded if the initial solution is smooth and satisfies the proper boundary conditions for $t = 0$.

3.2. Discretizations with DIRK methods

As we saw in the above example, stability properties of discretized forms of (1.3) can be better than for the continuous version. A natural way to obtain discretized forms is to use diagonally implicit Runge–Kutta (DIRK) methods, possibly together with continuous extensions (dense output formulas). Examples for such methods are found in [4,7] and below we shall use a simple second-order DIRK method for a numerical illustration.

We shall consider two approaches using DIRK methods. The first approach is based on continuous extensions, and different methods can be chosen for each equation in (1.3a), (1.3b). The second approach is to use one single DIRK method for the whole system (1.3). In all cases the step size for the DIRK methods will be chosen as $\tau = t_{n+1} - t_n$. Smaller sub-time steps could be taken, but formally that is the same as taking one step with some DIRK method with more stages.

Approach (A): The equations (1.3a), (1.3b) can be solved successively by continuous DIRK methods, producing approximations $\bar{V}_i(t)$ and $V_i(t)$ for $\bar{v}_i(t)$, $v_i(t)$, $i = 1, \ldots, m$, respectively. Note that the approximation $\bar{V}_i(t)$ will produce the source term $F_1(t, \bar{V}_i(t))$ for (1.3b), and likewise $V_{i-1}(t)$ will give the proper source term for equation (1.3a).

This approach is interesting, at least potentially, since different methods could be used for each Eq. (1.3a) and (1.3b). Hence the methods could be chosen only on the basis of their suitability to solve the particular sub-problem. However, in our attempts this approach did lead to schemes that become unstable if the stiffness is increased. An illustration is provided below. In view of the above example for θ-methods with $\theta_1 \neq \theta_2$ this unfavourable behaviour is not really surprising anymore.

Approach (B): Another possible implementation is to apply one DIRK method directly to the whole system (1.3) written out with $i = 1, \ldots, m$. If the DIRK methods has s stages, this leads directly to a splitting method with $2sm$

stages, each of which is implicit in either F_1 or F_2. The order of the scheme is then $p_m = \min(2m, p)$ where p is the order of the DIRK method itself. Continuous extensions are not needed here.

3.2.1. Numerical test with a two-stage DIRK method

For a numerical illustration we consider a simple two-stage DIRK method. Using the same Runge–Kutta notation as in [4, p. 100], the method is given by the Butcher tableau

$$\begin{array}{c|cc} c_1 & a_{11} & \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array} \quad = \quad \begin{array}{c|cc} \gamma & \gamma & \\ 1-\gamma & 1-2\gamma & \gamma \\ \hline & 1/2 & 1/2 \end{array} \tag{3.4}$$

with the continuous extension coefficients

$$b_1(\theta) = \frac{1}{2}\theta\,\frac{2-2\gamma-\theta}{1-2\gamma}, \quad b_2(\theta) = \frac{1}{2}\theta\,\frac{\theta-2\gamma}{1-2\gamma}. \tag{3.5}$$

For the step from t_n to t_{n+1} these coefficients will give approximations in $t_{n+\theta} = t_n + \theta\tau$, $\theta \in [0, 1]$, and for $\theta = 1$ we recover the weights $b_1 = \frac{1}{2}$, $b_2 = \frac{1}{2}$ of (3.4). Although in approach (A) different methods might be used for each Eq. (1.3a) and (1.3b), we consider here only the method with parameter value $\gamma = 1 + \frac{1}{2}\sqrt{2}$. With this parameter the DIRK method is L-stable, and both (3.4) and (3.5) are then second-order accurate.

The test problem is given by the reaction–diffusion equations

$$\begin{aligned} u_t &= D_1 u_{xx} - k_1 u + k_2 v + s_1(x), \\ v_t &= D_2 v_{xx} + k_1 u - k_2 v + s_2(x), \end{aligned} \tag{3.6}$$

for $0 < x < 1$ and $0 < t \leqslant T = \frac{1}{2}$, with initial- and boundary conditions

$$\begin{aligned} &u(x, 0) = 1 + \sin(\tfrac{1}{2}\pi x), \quad v(x, 0) = \frac{k_1}{k_2} u(x, 0), \\ &u(0, t) = 1, \quad v(0, t) = \frac{k_1}{k_2}, \quad u_x(1, t) = v_x(1, t) = 0. \end{aligned} \tag{3.7}$$

The parameters and source terms are set to

$$D_1 = 0.1, \quad D_2 = 0, \quad k_1 = 1, \quad k_2 = 10^4, \quad s_1(x) = 1, \quad s_2(x) = 0. \tag{3.8}$$

Further we use standard second-order differences for the spatial derivative with 100 grid points $x_j = jh$, $h = \frac{1}{100}$. This leads to an ODE system (1.1) of dimension $M = 200$. For the splitting we consider F_1 to be the discretized diffusion together with the inhomogeneous boundary condition, and F_2 denotes the reaction term plus source term. The errors for the splitting schemes are measured in the maximum norm (i.e., maximum over the two components and the grid points) at time T with respect to a time-accurate integration of the ODE system.

Table 1 gives the temporal errors of the iterated splittings with $m = 1$ and the two approaches: approach (A) (using dense output) and approach (B) (direct application of the DIRK method). Also results for a variant approach (A′) are

Table 1
Errors versus step size τ for the reaction–diffusion test

	Approach (A)	Approach (A′)	Approach (B)
$\tau = \frac{1}{10}$	$2.14 \cdot 10^{19}$	$6.67 \cdot 10^{17}$	$2.17 \cdot 10^{-3}$
$\tau = \frac{1}{20}$	$2.88 \cdot 10^{37}$	$2.81 \cdot 10^{34}$	$6.71 \cdot 10^{-4}$
$\tau = \frac{1}{40}$	$8.99 \cdot 10^{67}$	$8.56 \cdot 10^{61}$	$1.91 \cdot 10^{-4}$

added; here we take instead of the dense output formula (3.5) simply linear interpolation between t_n and t_{n+1} for any intermediate point $t_{n+\theta} = t_n + \theta\tau$. This is only first-order accurate, but it is the most stable interpolation possible.

We see that the direct approach (B) produces satisfactory results, but the approach (A) and its variant give huge errors. Moreover, it was observed that with smaller mesh widths h these errors become even larger. Therefore, we can conclude that the approach (A) is not stable for the case that eigenvalues of A_1 tend to $-\infty$. This is completely similar to formula (3.2) for the θ-methods with $\theta_1 \neq \theta_2$.

Taking $k_2 = 1$ (non-stiff reaction) did give essentially the same results. Only if we interchange reaction and diffusion, that is, F_1 being reaction plus source term and F_2 being discretized diffusion with boundary condition, then this case with non-stiff reaction produced good results for the approach (A) and (A′). We did not elaborate the stability functions for these schemes, but it is obvious from the numerical results that we will get an expression somewhat similar to (3.2) for $\theta_1 \neq \theta_2$, with a bounded behaviour in Z_2 and an unbounded behaviour in Z_1 if eigenvalues tend to $-\infty$.

The experiments for approach (A) were repeated with other methods, for example, the continuous DIRK method presented in [4, p. 100], but the results were essentially the same as for the two-stage method.

Finally we remark that the above linear test problem was set up such that for $D_1 \neq D_2$ the operators A_1 and A_2 do not commute. It turned out, however, that the instabilities already appeared with equal diffusion coefficients $D_1 = D_2 \neq 0$.

Remark 3.2. The DIRK method with approach (B) appears to be stable in this example, similar to (3.2) with $\theta_1 = \theta_2$. If we consider the linear, scalar test equation $u' = (\lambda_1 + \lambda_2)u$ and an s-stage Runge–Kutta method with coefficient matrix $A = (a_{ij}) \in \mathbb{R}^{s\times s}$, weight vector $b = (b_i) \in \mathbb{R}^s$ and $e = (1, 1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^s$, then after m iterations we will have $u_{n+1} = R_m(z_1, z_2)u_n$ with $z_k = \tau\lambda_k$ and stability function R_m. For $m = 1, 2$, it follows by some calculations that

$$R_1(z_1, z_2) = 1 + (z_1 + z_2)b^{\mathrm{T}}(I - z_1A)^{-1}(I - z_2A)^{-1}e, \tag{3.9}$$

$$R_2(z_1, z_2) = R_1(z_1, z_2) + z_1z_2(z_1 + z_2)b^{\mathrm{T}}(I - z_1A)^{-2}(I - z_2A)^{-2}A^2e, \tag{3.10}$$

which are the discrete counterparts of (2.6) and (2.7) with approach (B). However, a full analysis of these functions is still difficult. Since it will be clear from the following that we do not advocate these methods anyway, this issue will not be pursued here any further.

3.2.2. Relations with additive and fractional step Runge–Kutta methods

The above experiment has also been performed for approach (B) with higher order DIRK methods, in particular with $m = 2$, $s = 4$ and order $p = 4$. This gives in total 16 stages, eight of them implicit in F_1 and eight implicit in F_2. Again the results were good, with fourth-order convergence. So, in this respect the approach (B) seems interesting.

However, looking more carefully at schemes obtained in this way, it becomes clear that they are in fact special cases of the so-called fractional step Runge–Kutta methods. Stable schemes of this type with fewer stages than in the above construction are known; see [1,2]. Therefore, the schemes obtained in this way via the iterated splitting approach are not optimal in terms of number of stages versus the order of accuracy, and also stability is an issue that needs careful study.

For applications, the iterated splitting would have been more interesting if the discretizations of (1.3a) and (1.3b) could have been chosen only on the basis of their suitability to solve the particular sub-problem, but, as we saw, such attempts did lead to unstable schemes.

The above discussion on instabilities with iterated splittings applies to problems where both F_1 and F_2 give rise to stiffness, necessitating implicit treatment for both these terms. If F_1 is a non-stiff term, or a mildly stiff one, a better stability behaviour could be expected. However, also then the iterated splitting approaches would lead to schemes with many stages that seem not competitive with existing combinations of implicit and explicit methods; see for example the additive Runge–Kutta schemes presented in [7] or IMEX schemes based on multistep, Runge–Kutta or Rosenbrock methods [5].

4. Conclusions

At first sight, the iterated splitting scheme (1.3) seems to have some attractive features. For example, different Runge–Kutta methods might be employed for the different fractional steps, while maintaining consistency with the full system (1.1).

However, the stability properties of (1.3) turn out to be quite poor, even for simple linear systems without discretization of (1.3a) and (1.3b). This result already makes the iterated splitting less attractive for stiff systems.

Discretized forms with different methods for the different fractional steps (1.3a), (1.3b) turned out to be unstable in general.

Specific discretizations are possible that have better stability properties than the continuous system (1.3), but these lead to well-known splitting methods that are better studied in their own right without reference to (1.3).

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