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A note on splitting errors for advection–reaction equations

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Abstract

In this note we consider proper ways to combine numerical schemes for advective transport and nonlinear chemistry. Obvious combinations are obtained with splitting in a so-called fractional step approach. We shall discuss for this approach correct implementations of source terms and inflow boundary conditions. Further we consider the use of multistep methods with explicit treatment of the advection terms and implicit chemistry.

Keywords: Hyperbolic PDEs; Linear advection; Operator splitting

1. Introduction

Advective transport of chemically reacting species can be described by equations of the type

$$\frac{\partial}{\partial t}c + u(t, x) \cdot \nabla c = f(t, x, c) \qquad \text{for } t > 0, \quad x \in \Omega \subset \mathbb{R}^d, \tag{1.1}$$

where $c(t, x)$ is a vector of scaled chemical concentrations (mixing ratios), $u(t, x)$ is a given velocity field with dimension d, and $f(t, x, c)$ describes the chemical reactions together with source and sink terms. In our notation c will be treated as a scalar quantity, although in general $c \in \mathbb{R}^s$.

Suppose the advection operator is discretized in a suitable way, say by finite differences. Then (1.1) yields an ODE system

$$\frac{\mathrm{d}}{\mathrm{d}t}w(t) = A(t, w(t)) + F(t, w(t)), \tag{1.2}$$

where $w(t) = [w_i(t)]$ with vector-valued components $w_i(t) \in \mathbb{R}^s$ approximating the concentra-

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tion vector c at time t in the grid points x_i. Further, $A(t, w(t))$ represents the discretized advection operator and $F_i(t, w(t)) = f(t, x_i, w_i(t))$. Other discretizations, such as finite volumes or finite elements, give semidiscrete systems with similar interpretations. Usually, $A(t, w)$ will be linear in w, but it may become nonlinear if some form of limiting is used to avoid oscillations and negative values, see [5] for instance.

For the time integration of the advection part explicit methods are usually more efficient than implicit ones. On the other hand, the reaction equations are often very stiff, so this requires the use of implicit methods. To combine the preferred methods we consider *operator splitting*. Assuming the fully discrete approximation $w_n = [w_i^n]$ has been computed, with $w_i^n \approx w_i(t_n)$, $t_n = n\tau$, the next approximation is found by solving on the interval $[t_n, t_{n+1}]$ the fractional steps

$$\frac{\mathrm{d}}{\mathrm{d}t} w^*(t) = A(t, w^*(t)), \quad w^*(t_n) = w_n, \tag{1.3}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} w^{**}(t) = F(t, w^{**}(t)), \quad w^{**}(t_n) = w^*(t_{n+1}), \tag{1.4}$$

and setting

$$w_{n+1} = w^{**}(t_{n+1}). \tag{1.5}$$

Alternatively, one may also reverse the order of the fractional steps (1.3) and (1.4), that is, first perform chemistry and then advection. If we reverse the order of the subprocesses after each complete time step we get the symmetrical Strang splitting.

In such splitting procedures, at each fractional step a different time integration method can be chosen, implicit for the chemistry and explicit for the advection. Moreover, in the solution of the chemical equations (1.4) there is only coupling between the chemical components in each grid point separately, not over the grid points. Since accurate solution of stiff nonlinear systems is expensive in terms of computing time, this provides obvious opportunities for parallel computations.

In general, the simple splitting (1.3)–(1.4) introduces a splitting error of $O(\tau)$. One of the objects of this note is to show that the splitting error will disappear if (1.4) is slightly modified, such that space-dependent chemistry and source terms are integrated along characteristics, and no past information $t < t_n$ is used in the fractional steps. The appropriate characteristics that are to be used in this process are determined by the order of the fractional steps (i.e., advection first or reaction first).

Straightforward use of multistep methods to solve the fractional steps leads to a low order of accuracy (or even inconsistency, i.e., order zero). A better way to use multistep methods is to start with a multistep discretization for the total equation (1.2) and then to perform splitting *within* the time discretization. This will be discussed in Section 3.

In Section 4 the problem of specifying correct boundary conditions in the fractional step approach will be discussed. As we shall see, if the reaction is stiff and the inflow is not in chemical equilibrium, then it is advisable to interchange the order of the fractional steps (1.3)–(1.4).

2. Fractional steps with one-step and multistep methods

2.1. One-step methods

In the following it will be assumed that the spatial discretization has order q with mesh width h, and that the advection and reaction equations are solved with stable, consistent methods. Moreover, all arising functions will tacitly be assumed to be sufficiently smooth and $\|\cdot\|$ will denote some suitable norm. Further, in this section we take $\Omega=\mathbb{R}^d$, so that no boundary conditions are required.

The splitting errors for the advection–reaction equation can be very easily analyzed by interpreting (1.1) in physical terms, using the characteristics, see also LeVeque and Yee [6]. Consider

$$\bar{x}'(t)=u(t,\bar{x}(t)), \qquad \bar{x}(t_{n+1})=x_i, \tag{2.1}$$

with x_i a grid point, and let $\bar{x}_i=\bar{x}(t_n)$. If we set $\bar{c}(t)=c(t,\bar{x}(t))$ and $\bar{c}_i^n=c(t_n,\bar{x}_i)$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\bar{c}(t)=f(t,\bar{x}(t),\bar{c}(t)), \quad \bar{c}(t_n)=\bar{c}_i^n. \tag{2.2}$$

Hence, solving (1.1) can be done in two steps: first, compute $\bar{c}_i^n$, which amounts to solving the advection only, and then integrate the remaining reaction equation for $t_n\leqslant t\leqslant t_{n+1}$. In (1.3)–(1.4) the same is done with the semidiscrete system. We note that any method for solving advection can be interpreted as an interpolation scheme to approximate the values $\bar{c}_i^n$, see [8].

Theorem 2.1. *Suppose* (1.3) *and* (1.4) *are computed with one-step methods of order* p, *and* $f(t,x,c)$ *is independent of* x. *Then the global error can be bounded by*

$$\|c(x_i,t_n)-w_i^n\|=\mathrm{O}(\tau^p)+\mathrm{O}(h^q)$$

uniformly in i *and* n *for* $t_n\leqslant T$.

Proof. Suppose we start at $t=t_n$ with exact data. As observed above, computation of (1.3) will give approximations to $\bar{c}_i^n$ with an error of $\mathrm{O}(\tau^{p+1})+\mathrm{O}(\tau h^q)$. Further, since f is assumed to be independent of x, the fractional step (1.4) is equivalent with (2.2). Hence, the computation of (1.4) will just introduce an additional local error of $\mathrm{O}(\tau^{p+1})$. Since these are the errors which are introduced in one single step, the stability assumption gives the above bound for the global errors. □

Apart from stability, there are no conditions on the one-step method. So, this can either be a Runge–Kutta method or a direct method, such as Lax–Wendroff.

Next, suppose that f does depend on x, as will be the case if source terms are included with the reactions. Then (1.4) reads

$$\frac{\mathrm{d}}{\mathrm{d}t}w_i^{**}(t)=f(t,x_i,w_i^{**}(t)), \quad w_i^{**}(t_n)=w_i^{*}(t_{n+1}) \tag{2.3}$$

for all components i. However, in this way we introduce a first-order splitting error, or second-order when Strang splitting is used.

These splitting errors can be easily avoided by integrating the reaction term along the characteristics. So, we should replace (2.3) by

$$\frac{\mathrm{d}}{\mathrm{d}t} w_i^{**}(t) = f(t, x_i^{**}(t), w_i^{**}(t)), \quad w_i^{**}(t_n) = w_i^{*}(t_{n+1}), \tag{2.4}$$

where $x_i^{**}(t)$ is as in (2.1), i.e., the characteristic that passes at $t = t_{n+1}$ through the point x_i. In the same way as in Theorem 2.1 it is easily seen that there will be no splitting error when the fractional steps are computed with one-step methods.

The computation of these characteristics can be done with an explicit Runge–Kutta method or by a Taylor series. The amount of work involved with this is likely to be negligible compared to the work needed to solve the stiff reactions themselves.

In case the reaction step is performed prior to the advection step the same remains valid if we integrate the reaction term along $x_i^*(t)$, the characteristic that passes through x_i at time $t = t_n$. This follows from a similar reasoning, by tracing the characteristics forward in time, starting at time level t_n, so that now the w_i^n give the initial values for the chemistry step.

At first sight it might seem a bit strange that in order to find $c(t_{n+1}, x_i)$ we now use a characteristic that does not pass through (t_{n+1}, x_i) but through a downstream point $(t_{n+1}, x_i^*(t_{n+1}))$. However, if we first perform the reaction computation

$$\frac{\mathrm{d}}{\mathrm{d}t} w_i^{*}(t) = f(t, x_i^{*}(t), w_i^{*}(t)), \quad w_i^{*}(t_n) = w_i^{n} \tag{2.5}$$

over (t_n, t_{n+1}), the resulting $w_i^*(t_{n+1})$ should not be interpreted as an attempt to approximate $c(t_{n+1}, x_i)$ as good as possible—after all, there is still an advection step to follow.

Summarizing, the result of Theorem 2.1 remains valid if the reactions are integrated along the appropriate characteristics. So, with little extra effort the splitting error will disappear.

2.2. Linear multistep methods

As we shall see in this section, direct use of linear multistep methods to solve the fractional steps (1.3) and (1.4) gives a drop in accuracy. Since this happens already in case A and F are linear and constant in time, we only consider this simplest case.

With direct application of a linear multistep method to solve (1.3),

$$w_{n+1}^* + \sum_{j=1}^{k} \alpha_j w_{n+1-j} = \tau\beta_0 A w_{n+1}^* + \tau \sum_{j=1}^{k} \beta_j A w_{n+1-j}, \tag{2.6}$$

the conclusion of Theorem 2.1 is not valid, since the vector w_{n+1}^* should approximate the result of the step $t_n \mapsto t_{n+1}$ with advection only, whereas the past vectors w_{n+1-j}, $j = 2, \ldots, k$, are approximations of the full equation, i.e., advection with reaction. The extent to which this inconsistency influences the error depends on whether the method is of the Adams type or not.

Theorem 2.2. *Consider the splitting* (1.3)–(1.4) *and suppose that* (1.4) *is solved exactly or with a consistent one-step method, and that* (1.3) *is solved with the linear multistep method* (2.6). *Then the global temporal errors will be of* $\mathrm{O}(\tau)$ *if* $\alpha_j = 0$ $(j = 2, \ldots, k)$, *and of* $\mathrm{O}(1)$ *otherwise.*

Proof. Consider the formula

$$\tilde{w}_{n+1}^* + \sum_{j=1}^{k} \alpha_j w^*(t_{n+1-j}) = \tau\beta_0 A\tilde{w}_{n+1}^* + \tau \sum_{j=1}^{k} \beta_j A w^*(t_{n+1-j})$$

with $w^*(t)$ exact solution of (1.3). Obviously $\tilde{w}_{n+1}^*$ approximates $w^*(t_{n+1})$ with $O(\tau^{p+1})$ accuracy.

To consider the local error with (2.6), suppose that we start with exact values $w_k = w(t_k)$, $k \leqslant n-1$ of

$$\frac{\mathrm{d}}{\mathrm{d}t}w(t) = Aw(t) + Fw(t), \quad w(t_n) = w_n.$$

Using $w^*(t_n) = w(t_n)$ it follows that

$$\| w^*(t) - w(t) \| = O(t_n - t) \max_{t \leqslant s \leqslant t_n} \| Fw(s) \|$$

for $t_{n+1-k} \leqslant t \leqslant t_n$. Since

$$(I - \tau\beta_0 A)(\tilde{w}_{n+1}^* - w_{n+1}^*) = \sum_{j=1}^{k} (-\alpha_j + \tau\beta_j A)\big(w^*(t_{n+1-j}) - w_{n+1-j}\big),$$

we obtain the local error estimate

$$\| \tilde{w}_{n+1}^* - w_{n+1}^* \| = O(\tau^{\nu}) \max_{t \leqslant t_n} \| Fw(t) \|$$

with $\nu = 2$ if $\alpha_j = 0$ $(j = 2, \ldots, k)$, and $\nu = 1$ otherwise.

These are the local temporal errors, and thus globally we get temporal order one and zero, respectively. □

It is clear that the same low orders will be obtained if the reaction equations are solved with by a multistep method, such as BDF, assuming the advection part is solved exactly or with a consistent one-step method. In the next section we shall discuss a more appropriate way to implement BDF methods for the advection–reaction equations.

Example. As an illustration of Theorem 2.2, we consider

$$c_t + c_x = -10c, \qquad 0 \leqslant t \leqslant \tfrac{1}{2}, \quad 0 \leqslant x \leqslant 1 \tag{2.7}$$

with periodicity conditions at the boundaries, $c(t, 0) = c(t, 1)$, and with exact solution

$$c(t, x) = 1000\mathrm{e}^{-10t} \cos(\pi(x-t))^2. \tag{2.8}$$

Spatial discretization is performed with fourth-order central differences on a uniform grid with mesh width h, and for the time integration we consider the classical Runge-Kutta method and the three-step Adams method in PECE mode, see for instance [3]. Both methods are of order 4, but the Runge–Kutta method requires twice as much work per time step. To compensate for this we take step sizes $\tau = h$ for the Runge–Kutta method and $\tau = h/2$ for the Adams method. With splitting the "reaction equation" is solved exactly. Table 1 gives the relative L_2-errors at $t = \frac{1}{2}$ for both methods with and without splitting. Note that the Runge–Kutta method becomes

Table 1
L_2-errors of Runge–Kutta method ($\tau = h$) and Adams method ($\tau = h/2$) for (2.7)

	Runge–Kutta		Adams PECE	
	No splitting	Splitting	No splitting	Splitting
$h = 1/10$	0.14	$0.11 \cdot 10^{-1}$	$0.96 \cdot 10^{-1}$	$0.95 \cdot 10^{-1}$
$h = 1/20$	$0.62 \cdot 10^{-2}$	$0.72 \cdot 10^{-3}$	$0.46 \cdot 10^{-2}$	$0.57 \cdot 10^{-1}$
$h = 1/40$	$0.32 \cdot 10^{-3}$	$0.45 \cdot 10^{-4}$	$0.26 \cdot 10^{-3}$	$0.27 \cdot 10^{-1}$
$h = 1/80$	$0.18 \cdot 10^{-4}$	$0.28 \cdot 10^{-5}$	$0.15 \cdot 10^{-4}$	$0.14 \cdot 10^{-1}$

more accurate with splitting due to the insertion of the exact solution in the reaction step. The $O(\tau)$ behaviour with the associated degradation in accuracy for Adams method with splitting is clearly visible. With other multistep methods, for instance Leap-Frog, it would even become worse.

3. Splitting within multistep methods: implicit–explicit methods

Consider a multistep method, for instance BDF,

$$\sum_{j=0}^{k} \alpha_j w_{n+1-j} = \tau \sum_{j=0}^{k} \beta_j \big(A(t_{n+1-j}, w_{n+1-j}) + F(t_{n+1-j}, w_{n+1-j}) \big), \tag{3.1}$$

with implicit treatment of advection and chemistry. We can handle the advection explicitly by applying an extrapolation formula

$$v(t_{n+1}) = \sum_{j=1}^{k} \gamma_j v(t_{n+1-j}) + O(\tau^q) \tag{3.2}$$

with $v(t) = A(t, w(t))$. This leads to the method

$$\sum_{j=0}^{k} \alpha_j w_{n+1-j} = \tau \sum_{j=0}^{k} \beta_j F(t_{n+1-j}, w_{n+1-j}) + \tau \sum_{j=1}^{k} \delta_j A(t_{n+1-j}, w_{n+1-j}), \tag{3.3}$$

with new coefficients $\delta_j = \beta_j + \beta_0 \gamma_j$. Methods of this type are called implicit–explicit multistep methods, and they have been studied by Crouzeix [2], Varah [12] and Asher et al. [1] for parabolic equations and advection–diffusion problems.

Theorem 3.1. *Assume the implicit multistep method* (3.1) *has order p and the extrapolation procedure* (3.2) *has order q. Then method* (3.3) *has order* $r = \min(p, q)$.

Proof. The local truncation error for (3.3) can be written as

$$\frac{1}{\tau} \sum_{j=0}^{k} \big(\alpha_j w(t_{n+1-j}) - \tau \beta_j w'(t_{n+1-j}) \big) + \beta_0 \left(A(t_{n+1}, w(t_{n+1})) - \sum_{j=1}^{k} \gamma_j A\big(t_{n+1-j}, w(t_{n+1-j})\big) \right)$$

$$= C \tau^p \frac{\mathrm{d}^{p+1}}{\mathrm{d}t^{p+1}} w(t_n) + O(\tau^{p+1}) + C' \tau^q \frac{\mathrm{d}^q}{\mathrm{d}t^q} A(t_n, w(t_n)) + O(\tau^{q+1}),$$

with constants C and C' determined by the coefficients of the multistep method and the extrapolation procedure. □

The most simple method of the type (3.3) reads

$$w_{n+1} = w_n + \tau A(t_n, w_n) + \tau F(t_{n+1}, w_{n+1}). \tag{3.4}$$

This method is also obtained with the fractional step approach if we use the forward Euler method in (1.3) and the backward Euler method in (1.4). Methods with $k > 1$ are essentially different from fractional step methods.

Example. For the BDF2 method with quadratic extrapolation, we get the second-order scheme

$$w_{n+1} - \tfrac{4}{3}w_n + \tfrac{1}{3}w_{n-1} = \tfrac{2}{3}\tau\big(2A(t_n, w_n) - A(t_{n-1}, w_{n-1})\big) + \tfrac{2}{3}\tau F(t_{n+1}, w_{n+1}), \tag{3.5}$$

and BDF3 with cubic extrapolation leads to the third-order scheme

$$\begin{aligned} &w_{n+1} - \tfrac{18}{11}w_n + \tfrac{9}{11}w_{n-1} - \tfrac{2}{11}w_{n-2} \\ &\quad = \tfrac{6}{11}\tau\big(3A(t_n, w_n) - 3A(t_{n-1}, w_{n-1}) + A(t_{n-2}, w_{n-2})\big) + \tfrac{6}{11}\tau F(t_{n+1}, w_{n+1}). \end{aligned} \tag{3.6}$$

The stability of such implicit–explicit methods is more complicated than for standard multistep methods. If we assume that A and F are linear with constant coefficients, commuting and "close" to normal, we can make an eigenvalue analysis, see [1,13]. We note that if the chemistry is linear and independent of x, then A and F will indeed commute; this is closely related to the fact that there is no splitting error in such a situation, see Theorem 2.1. Tests with the BDF2 method and quadratic extrapolation, combined with an upwind-biased space discretization, gave promising results in [13].

4. Boundary conditions for the fractional steps

In this section we discuss the proper boundary conditions for the splitting schemes. For the implicit–explicit multistep methods we can simply apply the given boundary conditions. For the fractional step method (1.3)–(1.4), however, modifications are required to maintain accuracy.

We assume that Dirichlet conditions are given at inflow boundaries. These are, of course, conditions for the whole problem (1.1). However, in the advection step (1.3) we need conditions for the advection equation only. The inflow conditions can be thought of as originating from a problem on a larger spatial domain. By the interpretation with the characteristics, see Section 2, it follows that we get a fully consistent treatment if the given boundary condition at time $t_n + \theta\tau$ are modified such that the reaction is "undone" for a time $\theta\tau$, that is, the boundary terms should be integrated with chemistry *backwards* in time over $[t_n, t_n + \theta\tau]$. If the reaction is stiff, which it usually is, this may introduce numerical difficulties since stiff problems are unstable if time is reversed.

A way to avoid this backward integration is to perform splitting with first reaction and then advection. In this case we use input values $w_i^{**}(t_n)$ for the advection step that have already been subjected to the chemistry on $[t_n, t_{n+1}]$. It follows that a given boundary condition at time $t_n + \theta\tau$ should be integrated forward in time, with chemistry only, on the interval $[t_n + \theta\tau, t_{n+1}]$, to give a fully consistent treatment within the splitting process.

Table 2
Relative L_2-errors for (4.1) at $t = 1/2$

	Simple splitting	Strang splitting	Corrected boundary
$\tau = 1/10$	$0.52 \cdot 10^{-1}$	$0.25 \cdot 10^{-1}$	$0.99 \cdot 10^{-2}$
$\tau = 1/20$	$0.26 \cdot 10^{-1}$	$0.14 \cdot 10^{-1}$	$0.88 \cdot 10^{-3}$
$\tau = 1/40$	$0.14 \cdot 10^{-1}$	$0.48 \cdot 10^{-2}$	$0.91 \cdot 10^{-4}$
$\tau = 1/80$	$0.72 \cdot 10^{-2}$	$0.17 \cdot 10^{-2}$	$0.13 \cdot 10^{-4}$

Example. Consider the model advection–reaction equation

$$c_t + c_x = c^2, \qquad 0 \leqslant x \leqslant 1, \quad 0 \leqslant t \leqslant \tfrac{1}{2}, \tag{4.1}$$

with given initial value at $t = 0$ and Dirichlet condition at $x = 0$, derived from the exact solution

$$c(t, x) = \frac{\sin(\pi(x - t))^2}{1 - t \sin(\pi(x - t))^2}.$$

Spatial discretization is performed with fourth-order central differences in the interior and third-order one-sided approximations at the boundaries. The advection step is solved with the classical Runge–Kutta method at Courant number $\tau/h = 2$, and the "reaction" $c_t = c^2$ is solved exactly.

We consider:

(i) simple splitting (with reaction followed by advection) where in the advection step the given boundary values are used;

(ii) a Strang-type splitting [10] where after each time step the order of the fractional steps is reversed, also with the given boundary conditions;

(iii) the same splitting as in (*i*) but with corrected boundary conditions

$$c^{**}(t, 0) = \frac{c(t, 0)}{1 - (t_{n+1} - t)c(t, 0)} \quad \text{for } t \in [t_n, t_{n+1}].$$

The errors in the L_2-norm are given in Table 2.

The convergence rate of the method with boundary corrections is less than 4, but this is due to order reduction of the Runge–Kutta method (see [7]), it is not caused by the splitting procedure. A similar order reduction can be observed with Strang splitting: in the absence of boundary conditions it has (at least) order 2, but in the above table an order 1.5 behaviour can be observed.

5. Concluding remarks

Both approaches discussed in this paper, the fractional step approach and the implicit-explicit multistep approach, have certain advantages. It will depend on the actual application which approach is to be preferred.

With the implicit–explicit multistep method it is easy to include diffusion without loss of accuracy, see [13]. Diffusion with a fractional step approach can be included with a Strang-type splitting, but this will introduce an $O(\tau^2)$ error, with a constant proportional to the magnitude of the diffusion coefficient. A similar situation will arise if the advection is in conservation form with a velocity field that is not divergence-free; then the splitting error will be proportional to the divergence of u.

In the fractional steps, the step sizes for the subprocesses need not be the same. So, if there is much chemical activity on only a small part of the computational domain, we can use there smaller substep sizes for the chemistry on the interval $[t_n, t_{n+1}]$.

The fractional step approach is more flexible with respect to the choice of the advection scheme. One may use, for example, a further splitting in the advection step as in [4,9].

Finally we note that with both approaches the spatial and temporal resolution near sharp fronts has to be sufficiently high if the chemistry is very stiff, otherwise the behaviour may become qualitatively wrong, see [6]. Some form of local grid refinement, for example as in [11], therefore can be essential for stiff advection–reaction problems.

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