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A generalization of Peaceman–Rachford fractional step method

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Abstract

In this paper we develop a set of time integrators of type fractional step Runge–Kutta methods which generalize the time integrator involved in the classical Peaceman–Rachford scheme. Combining a time semidiscretization of this type with a standard spatial discretization, we obtain a totally discrete algorithm capable of discretizing efficiently a general parabolic problem if suitable splittings of the elliptic operator are considered. We prove that our proposal is second order consistent and stable even for an operator splitting in m terms which do not necessarily commute. Finally, we illustrate the theoretical results with various applications such as alternating directions or evolutionary domain decomposition.

Keywords: Fractional steps; Alternating direction implicit methods; Peaceman and Rachford; Domain decomposition

1. Introduction

During the last five decades many schemes under the general names of alternating direction, splitting or fractional step methods have been developed for solving efficiently multidimensional evolution problems of mathematical physics. Such methods have been revealed as a great contribution for solving complicated models in hydrodynamics, meteorology, oceanology, ecology, etc. The first method of this class can be found in the papers of Douglas [4] and Peaceman and Rachford [8]. In these works the authors analyze

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the main drawbacks of classical discretization methods for parabolic problems in the multidimensional (in space) case. Concretely, they choose the classical two-dimensional heat flow equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}, \tag{1}$$

together with homogeneous Dirichlet boundary conditions on a square and a suitable initial condition such that the resultant IBVP has a sufficiently smooth solution. For this simple problem the classical explicit method consists of solving the following difference equations:

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\tau} = \frac{u_{i-1,j}^{n} - 2u_{i,j}^{n} + u_{i+1,j}^{n}}{h^2} + \frac{u_{i,j-1}^{n} - 2u_{i,j}^{n} + u_{i,j+1}^{n}}{h^2},$$

where $u_{i,j}^{n} \approx u(t_0 + n\tau, x_0 + ih, y_0 + jh)$, being τ the time step and h the size of the spatial mesh.

It is well known that this scheme, which is convergent of first order in time and of second order in space, has a really low computational cost per time step but it has the drawback of being conditionally stable under the restriction $\tau \leqslant h^2/4$; this implies a very slow time integration when h is small. The previous restriction on the size of τ arising from stability can be removed by the use of an implicit scheme in which the second order derivatives are approximated by second differences evaluated in terms of the unknown in t_{n+1}:

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\tau} = \frac{u_{i-1,j}^{n+1} - 2u_{i,j}^{n+1} + u_{i+1,j}^{n+1}}{h^2} + \frac{u_{i,j-1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j+1}^{n+1}}{h^2}.$$

This classical scheme, which is also first order consistent in time and second order in space, is unconditionally stable but has the drawback of requiring the resolution of a large block tridiagonal linear system per time step if fine spatial meshes are used. It is well known that direct methods, as for example Gauss elimination procedure, are not appropriate to solve such systems since they fill with a lot of non null coefficients the originally sparse matrices. This forces us to use iterative processes for their resolution and to assume the increase in cost derived from a slow speed of convergence in many cases.

In 1955 Peaceman and Rachford proposed in [8] the following numerical method:

$$\begin{aligned}
\frac{u_{i,j}^{n+(1/2)} - u_{i,j}^{n}}{\tau/2} &= \frac{u_{i-1,j}^{n+(1/2)} - 2u_{i,j}^{n+(1/2)} + u_{i+1,j}^{n+(1/2)}}{h^2} + \frac{u_{i,j-1}^{n} - 2u_{i,j}^{n} + u_{i,j+1}^{n}}{h^2}, \\
\frac{u_{i,j}^{n+1} - u_{i,j}^{n+(1/2)}}{\tau/2} &= \frac{u_{i-1,j}^{n+(1/2)} - 2u_{i,j}^{n+(1/2)} + u_{i+1,j}^{n+(1/2)}}{h^2} + \frac{u_{i,j-1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j+1}^{n+1}}{h^2}.
\end{aligned} \tag{2}$$

Such scheme consists of two difference equations, the first one implicit in x direction and the second one in y direction, which are alternately used. It is well known that (2) is unconditionally stable and consistent of second order in both time and space and, moreover, it leads us to two tridiagonal systems per time step τ which can be solved easily using direct methods and in a parallel way.

The general alternating direction technique (see [6]) is based on decomposing the elliptic operator containing the spatial derivatives as the addition of as many terms as the number of spatial variables taking part in our problem. Then we group into each term the derivatives with respect to just one of the spatial variables and the key of the efficiency of an alternating direction implicit method is that in each internal stage only one of these simpler operators acts implicitly. This reduces the classical multidimensional problems to essentially one-dimensional problems, one per internal stage.

Fractional step methods (see [14]) can be considered as a generalization of the previous ideas. In such schemes, the differential elliptic operator is decomposed as an addition of an arbitrary number m of "simpler" operators, where m is not necessarily equal to the number of spatial variables and the operator splitting is not necessarily done by directions. In fact, in parabolic problems with more complicated geometries and/or more complicated spatial differential operators, it is very useful (in terms of reducing the computation time of the resultant algorithm) to consider an operator splitting subordinated to a suitable decomposition of the spatial domain (see [7]). This technique provides an algorithm of type domain decomposition which means that the linear systems involved in every time step can be solved in parallel, and besides, in comparison with the classical domain decomposition technique (see [9]), this technique has the advantage of avoiding the iterations needed in the classical option due to the overlaps of the domains (Schwarz iterations).

Revising classical literature concerning fractional step methods (see compendia [6,14]) there are only two classical schemes which satisfy suitable absolute stability properties for the case of an operator splitting in an arbitrary number m of terms that do not necessarily commute. They are the fractionary implicit Euler scheme (5) with m implicit internal stages, which is convergent of first order, and the two-cycle method (6) with $2m$ implicit internal stages, which has second order of convergence.

In this paper, we propose a second order stable time integrator with $2m - 2$ implicit stages. Its combination with a standard spatial discretization provides an unconditionally convergent totally discrete scheme for the numerical resolution of a general parabolic problem. It has two main advantages with respect to the two-cycle scheme: it is cheaper because it has less implicit stages and it belongs to the class of fractional step Runge–Kutta (FSRK) schemes introduced in [2]. The fact that it is included into the set of FSRK methods permits us to develop an easier study of its consistency and stability as well as to avoid in a simple way the phenomenon called order reduction which appears in the case of considering time dependent boundary conditions (see [12]). We want to remark that in the case $m = 2$, if we choose an operator splitting of (1) of type alternating directions together with a standard central difference spatial discretization, our proposal coincides with the classical Peaceman–Rachford method; this is one of the reasons why our scheme can be considered as a generalization of this celebrated alternating direction method. The other main reason is based in the fact that the stability result obtained for our method coincides with the obtained one for the Peaceman–Rachford scheme (A-stability in the same type of norms both for commutative and non-commutative operators). On the other hand, if we focus on the comparisons which we did previously between our method and the two-cycle scheme, our new proposal can also be considered as an improvement of such classical scheme.

The contents of the rest of the paper are organized as follows: the second section is devoted to the description of a general parabolic initial boundary value problem and the new method which we propose to solve it numerically, the convergence of this new method is proven in the next section through the study

of its consistency and stability and we include a last section where the theoretical results are illustrated with various numerical examples.

2. General formulation: the problem and the method

Let us consider the following operational formulation for a general linear parabolic initial boundary value problem whose coefficients may depend on time: Find $u : [t_0, T] \to \mathscr{H}$ such that

$$\begin{cases} \dfrac{\mathrm{d}u}{\mathrm{d}t} = A(t)u + f(t), \quad t \in (t_0, T], \\ Bu(t) = g(t) \in \mathscr{H}^b, \quad t \in (t_0, T], \quad u(t_0) = u_0 \in \mathscr{H}. \end{cases} \tag{3}$$

Here $(\mathscr{H}, \|.\|, \langle ., . \rangle)$ and $(\mathscr{H}^b, \|.\|_b, \langle ., . \rangle_b)$ are two Hilbert spaces. For each $t \in [t_0, T]$, $A(t) : \mathscr{D} \subseteq \mathscr{H} \to \mathscr{H}$ is an unbounded elliptic differential operator and $B : \mathscr{D} \subseteq \mathscr{H} \to \mathscr{H}^b$ is an abstract trace operator which determines the type of boundary conditions considered (Dirichlet, Neumann, Robin, …); notice that the fact that B is independent of t means that the boundary condition does not vary of type in time. We denote with $f(t)$ the source term, u_0 is the initial condition and $g(t)$ are the boundary data. We assume that all these data are sufficiently regular and compatible in order to guarantee that $u(t)$ is sufficiently smooth both in space and time directions.

Let us consider a partition in m terms for operators $A(t)$: $A(t) = \sum_{i=1}^{m} A_i(t)$, where $A_i(t) : \mathscr{D}_i \subseteq \mathscr{H} \to \mathscr{H}$ and $\mathscr{D} = \bigcap_{i=1}^{m} \mathscr{D}_i$, and also a partition in m smooth terms for the source term $f(t) = \sum_{i=1}^{m} f_i(t)$. Let us also use a decomposition of operator B in m new boundary operators of its same type $B_i : \mathscr{D}_i \subseteq \mathscr{H} \to \mathscr{H}_i^b$ in such a way that $\mathrm{Ker}\, B = \bigcap_{i=1}^{m} \mathrm{Ker}\, B_i$ and such that, for any $c > 0$, the following elliptic problems $\{(\mathscr{I} - cA_i)\, v = w \in \mathscr{H},\ B_i v = v_b \in \mathscr{H}_i^b\}$ have a unique solution which depends continuously on the data w and v_b.

There are two classical ways of developing and analyzing a numerical algorithm for solving problem (3). Both options consist of a suitable time integration process, similar to the classical discretization methods for ODEs, combined with a discretization technique for the spatial variables typical for elliptic problems. The main difference between them is the order in which these processes are considered and it has implications in the convergence analysis of the numerical algorithm. In this paper, we consider that problem (3) is firstly discretized in time and then the resulting family of elliptic boundary value problems is discretized in space. For example, the Peaceman–Rachford method can also be seen as the result of applying firstly the following time semidiscretization to problem (1):

$$\begin{cases} \begin{cases} U_n^j = U_n^{j-1} + \dfrac{\tau}{2} \displaystyle\sum_{k=j-1}^{j} (A_{i_k}(t_{n,k}) U_n^k + f_{i_k}(t_{n,k})), \\ B_{i_j} U_n^j = g(t_{n,j}), \quad j = 2, 3, \ \text{with } U_n^1 = u_n, \end{cases} \\ u_{n+1} = U_n^3, \quad n = 0, 1, \ldots, n_f - 1 \ \left(\text{with } n_f \equiv \left[\dfrac{T}{\tau} \right] \right), \end{cases} \tag{4}$$

where $t_{n,i} = t_n + (i-1)(\tau/2)$, for $i = 1, 2, 3$, $i_1 = i_3 = 1$, $i_2 = 2$, $A_1(t) = \partial^2/\partial y^2$, $A_2(t) = \partial^2/\partial x^2$, $f_1(t) \equiv f_2(t) \equiv 0$; a central difference discretization of the elliptic problems of (4) give us this well-known numerical algorithm. U_n^i, $i = 1, 2, 3$, denote the internal stages of the method and u_n denotes the semidiscrete numerical approximation to the exact solution in time $t_n = t_0 + n\tau$, i.e., $u_n(x, y) \approx$

$u(t_n, x, y)$. With this formulation, we notice that the classical Peaceman–Rachford scheme admits a natural generalization which permits us to use this method for the time integration of more general parabolic problems like (3) (not just the classical heat flow equation). It is also interesting to notice that other spatial discretization processes can be considered, not only of type finite differences (like in (2)), but also finite element discretizations (see [11]) or spectral methods (see [1]) among others. Furthermore, it can be proven that (4) can be applied in the case of considering an operator splitting as the addition of two simpler operators which do not necessarily commute. Thinking of more general applications of fractional step methods it seems logical to consider non-commuting splittings in an arbitrary number of terms. Looking for classical methods designed for operator splittings in any number of non-commutative operators, only two schemes can be found in the literature (see [6]). These methods are the fractionary implicit Euler scheme

$$\begin{cases} \begin{cases} U_n^j = U_n^{j-1} + \tau(A_j(t_{n+1})U_n^j + f_j(t_{n+1})), \\ B_j U_n^j = g(t_{n+1}) \qquad j = 1, \ldots, m, \ \text{with } U_n^0 = u_n, \end{cases} \\ u_{n+1} = U_n^m, \ n = 0, 1, \ldots, n_f - 1, \end{cases} \tag{5}$$

which is convergent of first order and the second order two-cycle scheme

$$\begin{cases} \begin{cases} U_n^j = U_n^{j-1} + \dfrac{\tau}{4} \displaystyle\sum_{k=j-1}^{j} (A_{i_j}(t_{n,k})U_n^k + f_{i_j}(t_{n,k})), \\ B_{i_j} U_n^j = g(t_{n,j}), \qquad j = 2, 3, \ldots, 2m+1, \ \text{with } U_n^1 = u_n, \end{cases} \\ u_{n+1} = U_n^{2m+1}, \ n = 0, 1, \ldots, n_f - 1, \end{cases} \tag{6}$$

where $i_j = j - 1$ if $2 \leqslant j \leqslant m+1$, $i_j = 2m + 2 - j$ if $m + 2 \leqslant j \leqslant 2m + 1$ and the intermediate times are $t_{n,1} = t_n$, $t_{n,i} = t_n + (\tau/2)$, $i = 2, \ldots, 2m$, $t_{n,2m+1} = t_n + \tau$.

For the same purposes, in this paper we introduce the following new method:

$$\begin{cases} \begin{cases} U_n^j = U_n^{j-1} + \tau \displaystyle\sum_{k=j-1}^{j} d_k \, (A_{i_k}(t_{n,k})U_n^k + f_{i_k}(t_{n,k})), \\ B_{i_j} U_n^j = g(t_{n,j}) \qquad j = 2, 3, \ldots, 2m-1, \ \text{with } U_n^1 = u_n, \end{cases} \\ u_{n+1} = U_n^{2m-1}, \ n = 0, 1, \ldots, n_f - 1, \end{cases} \tag{7}$$

where $i_j = j$ if $1 \leqslant j \leqslant m$, $i_j = 2m - j$ if $m + 1 \leqslant j \leqslant 2m - 1$. The intermediate times are $t_{n,1} = t_n$, $t_{n,j} = t_n + (\tau/2)$ (for $j = 2, 3, \ldots, 2m-2$), $t_{n,2m-1} = t_n + \tau = t_{n+1}$ and the coefficients considered are $d_1 = d_m = d_{2m-1} = \frac{1}{2}$, $d_j = \frac{1}{4} \ \forall \, j \in \{2, \ldots, m-1\} \cup \{m+1, \ldots, 2m-2\}$.

Following the previous ideas, we come to a totally discrete scheme combining the previous time integration with a suitable spatial discretization. It is clear that comparing method (7) consisting of m levels with a two cycle (6) with the same number m of levels our proposal is cheaper since it has two implicit stages less.

Notice that the time integrator involved in the classical Peaceman–Rachford scheme is a particular case of our proposal since we obtain (4) if we consider $m = 2$ in (7).

3. Convergence analysis

The analysis of the convergence of the method proposed here is performed by separating suitably the contributions of the time integration and the spatial discretization processes to the global error. From

now on C denotes a generic constant independent of the time step τ and the mesh size h. To carry out the analysis of the time semidiscretization proposed, we use that (7) is a time discretization procedure which can be included into the set of FSRK methods. Such schemes can be formulated as follows:

$$\begin{cases} \begin{cases} U_n^j = u_n + \tau \sum_{k=1}^{j} a_{jk}^{i_k}(A_{i_k}(t_{n,k})U_n^k + f_{i_k}(t_{n,k})), \\ B_{i_j} U_n^j = g(t_{n,j}), \end{cases} & j = 1, \ldots, s, \\ u_{n+1} = u_n + \tau \sum_{j=1}^{s} b_j^{i_j}(A_{i_j}(t_{n,j})\, U_n^j + f_{i_j}(t_{n,j})), & n = 0, 1, \ldots, n_f - 1, \end{cases} \tag{8}$$

being $i_\bullet \in \{1, \ldots, m\}$ and $t_{n,k} = t_n + c_k\tau$. It is clear that the calculus of the jth internal stage consists of solving the following elliptic boundary value problem $\{(\mathcal{I} - \tau a_{jj}^{i_j} A_{i_j}(t_{n,j}))U_n^j = F_{n,j},\ B_{i_j} U_n^j = g(t_{n,j})\}$, where $F_{n,j}$ is computed from the data of problem (3) and certain calculations from the previous internal stages. The main advantage provided by these methods, compared to classical semiimplicit methods, is that the operator implicitly involved in the calculation of the jth internal stage of an FSRK method is $A_{i_j}(t)$, whereas in classical implicit methods it is $A(t)$. Therefore, if operators $\{A_i(t)\}_{i=1}^m$ are simpler, in a sense, than $A(t)$, the linear systems coming from the combination of a method of this type with a suitable spatial discretization will be easier to solve. This facility will come from different causes depending on the type of splitting chosen for the operators $A(t)$. For example, if we choose a decomposition of type alternating directions for the elliptic operator involved in a multidimensional problem and we combine it with a suitable space discretization, we will reduce the problem to a set of systems with a structure close to be essentially one dimensional (e.g. tridiagonal), much simpler than the classical structure of the systems involved in classical implicit methods (e.g. block tridiagonal). On the other hand, if we choose a splitting related to a suitable decomposition of the spatial domain (see [7]), we come to a set of uncoupled linear systems per stage which can be solved simultaneously using parallel processors. FSRK methods (8) fit in the class of additive RK methods using the following formulation:

$$\begin{cases} \begin{cases} U_n^j = u_n + \tau \sum_{i=1}^{m} \sum_{k=1}^{s} a_{jk}^{i}(A_i(t_{n,k})\, U_n^k + f_i(t_{n,k})), \\ B_{i_j} U_n^j = g(t_{n,j}), \end{cases} & j = 1, \ldots, s, \\ u_{n+1} = u_n + \tau \sum_{i=1}^{m} \sum_{j=1}^{s} b_j^i(A_i(t_{n,j})U_n^j + f_i(t_{n,j})), & n = 0, 1, \ldots, n_f - 1, \end{cases}$$

by simply considering many additional null coefficients ($a_{jk}^i = 0$ for $i \neq i_k$, $b_k^i = 0$ for $i \neq i_k$ and $a_{jk}^i = 0$ for $k > j$). In order to organize the coefficients of a method of this type in an easily comprehensible formula it is useful to resort to the following generalization of the Butcher table notations:

$$\begin{array}{c|c|c|c|c} c & \mathcal{A}_1 & \mathcal{A}_2 & \ldots & \mathcal{A}_m \\ \hline & b_1^T & b_2^T & \ldots & b_m^T \end{array} \quad \left(c \equiv (c_j),\ b_i \equiv (b_j^i) \in \mathbb{R}^s,\ \mathcal{A}_i \equiv (a_{jk}^i) \in \mathbb{R}^{s\times s}\right).$$

3.1. Consistency

An FSRK method is said to be consistent of order p if its local error in time t_{n+1}, defined by $\rho_{n+1} = u(t_{n+1}) - \breve{u}_{n+1}$, where $\breve{u}_{n+1}$ is the numerical solution obtained after one step of (8) starting from the exact solution in the previous time moment ($\breve{u}_n = u(t_n)$), satisfies that $\rho_{n+1} = \mathcal{O}(\tau^{p+1})$. The necessary and

sufficient conditions which an FSRK method must satisfy to be consistent of order p when it is applied to solve a problem of type (3) are proven in [2]. In particular, an FSRK scheme is second order consistent if and only if its coefficients satisfy

$$b_i^{\mathrm{T}} e = 1, \quad b_i^{\mathrm{T}} c = \tfrac{1}{2}, \quad b_i^{\mathrm{T}} \mathscr{A}_j e = \tfrac{1}{2} \quad \forall i, j \in \{1, \ldots, m\}, \tag{9}$$

where $e = (1, \ldots, 1) \in \mathbb{R}^s$. Using these order conditions and taking into account that our method, using Butcher notations, corresponds to the following vectors and matrices (belonging to $\mathbb{R}^{2m-1}$ and $\mathbb{R}^{(2m-1)\times(2m-1)}$, respectively):

$$c = (0, \tfrac{1}{2}, \ldots, \tfrac{1}{2}, 1)^{\mathrm{T}}, \quad b_1 = (\tfrac{1}{2}, 0, \ldots, 0, \tfrac{1}{2})^{\mathrm{T}}, \quad b_2 = (0, \tfrac{1}{2}, 0, \ldots, 0, \tfrac{1}{2}, 0)^{\mathrm{T}}, \ \ldots,$$

$$b_{m-1} = (\underbrace{0, \ldots, 0}_{m-2}, \tfrac{1}{2}, 0, \tfrac{1}{2}, \underbrace{0, \ldots, 0}_{m-2})^{\mathrm{T}}, \quad b_m = (\underbrace{0, \ldots, 0}_{m-1}, 1, \underbrace{0, \ldots, 0}_{m-1})^{\mathrm{T}},$$

$$\mathcal{A}_1 = \begin{pmatrix} 0 & & & & \\ \frac{1}{2} & 0 & & & \\ \vdots & \vdots & \ddots & & \\ \frac{1}{2} & 0 & \ldots & 0 & \\ \frac{1}{2} & 0 & \ldots & 0 & \frac{1}{2} \end{pmatrix}, \quad \mathcal{A}_2 = \begin{pmatrix} 0 & & & & & \\ 0 & \frac{1}{4} & & & & \\ 0 & \frac{1}{2} & 0 & & & \\ \vdots & \vdots & \vdots & \ddots & & \\ 0 & \frac{1}{2} & 0 & \ldots & 0 & \\ 0 & \frac{1}{2} & 0 & \ldots & 0 & \frac{1}{4} \\ 0 & \frac{1}{2} & 0 & \ldots & 0 & \frac{1}{2} & 0 \end{pmatrix}, \quad \ldots,$$

$$\mathcal{A}_{m-1} = \begin{pmatrix} 0 & & & & & & & \\ \vdots & \ddots & & & & & & \\ 0 & \ldots & 0 & & & & & \\ 0 & \ldots & 0 & \frac{1}{4} & & & & \\ 0 & \ldots & 0 & \frac{1}{2} & 0 & & & \\ 0 & \ldots & 0 & \frac{1}{2} & 0 & \frac{1}{4} & & \\ 0 & \ldots & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\ \underbrace{0 \ \ldots \ 0}_{m-2} & & & \frac{1}{2} & 0 & \frac{1}{2} & \underbrace{0 \ \ldots \ 0}_{m-2} & \end{pmatrix}, \quad \mathcal{A}_m = \begin{pmatrix} 0 & & & & & & \\ \vdots & \ddots & & & & & \\ 0 & \ldots & 0 & & & & \\ 0 & \ldots & 0 & \frac{1}{2} & & & \\ 0 & \ldots & 0 & 1 & 0 & & \\ \vdots & & \vdots & \vdots & \vdots & \ddots & \\ \underbrace{0 \ \ldots \ 0}_{m-1} & & & 1 & \underbrace{0 \ \ldots \ 0}_{m-1} & & \end{pmatrix}$$

it is not difficult to prove the following result:

Theorem 3.1. *The method* (7) *satisfies the second order conditions* (9) *for any number m of levels.*

Nevertheless, as it happens with many classical time integrators (see [13]) and also with the classical Peaceman–Rachford method (see [5]), in the case of considering time-dependent boundary conditions an order reduction occurs in our method from the classical order 2 to the order of the internal stages q, where q is the largest integer satisfying $j\mathscr{A}_i\mathscr{C}^{j-1}e = \mathscr{C}^j e$, $\forall i \in \{1, \ldots, m\}$, $\forall j \in \{1, \ldots, q\}$,

with $\mathscr{C} = \mathrm{diag}(c_1, \ldots, c_s) \in \mathbb{R}^{s\times s}$. Notice that $q = 0$ for our proposal (7) except for $m = 2$ (case of Peaceman–Rachford method), where $q = 1$. Fortunately, techniques to avoid the order reduction have been developed recently for general FSRK methods, which obviously can be used for this new method too. As it happens with classical time integrators, this order reduction is caused by the fact that the classical election for the boundary conditions for the internal stages, which consists of evaluating the boundary data in the intermediate times $t_{n,j}$, i. e., $B_{i_j} U_n^j = g(t_{n,j})$, is not the most appropriate one (see [12]). The way of improving the boundary conditions is based in considering the following auxiliary iterations:

$$\widehat{U}_n^{[0]} = (u(t_{n,1}), \ldots, u(t_{n,s}))^{\mathrm{T}},$$

$$\widehat{U}_n^{[l]} = eu(t_n) + \tau \sum_{i=1}^{m} \mathscr{A}_i (\widehat{A}_i^n \widehat{U}_n^{[l-1]} + \widehat{F}_i^n), \quad l \geqslant 1,$$

where $\widehat{A}_i^n = \mathrm{diag}(A_i(t_{n,1}), \ldots, A_i(t_{n,s}))$, $\widehat{F}_i^n = (f_i(t_{n,1}), \ldots, f_i(t_{n,s}))^{\mathrm{T}}$ and in choosing $B_{i_j} U_n^j = B_{i_j} \widehat{U}_n^{[l],j}$ ($\widehat{U}_n^{[l],j}$ denotes the jth component of vector $\widehat{U}_n^{[l]}$) if we want to recover l units of the lost order. We want to remark that these modifications are very easy to include in a standard code and that the increase of the computational cost of the modified algorithm is negligible (see [12] for more details).

Using the theoretical results which appear in [12], it is deduced for our method that, if operators $\{A_i(t)\}_{i=1}^m$ commute, then $\|\rho_n^{[l]}\| \leqslant C\tau^{\overline{q}[l]+1}$, where $\rho_n^{[l]}$ is the local error obtained with our semidiscrete scheme, considering boundary conditions improved l times for the internal stages, and $\overline{q}[l] = \min\{2, q + l\}$. For the non-commutative case, it can be proven in a similar way that this local error satisfies $\|\rho_n^{[l]}\|_{1,t_n} \leqslant C\tau^{\overline{q}[l]+1}$, where $\|v\|_{1,t} = \|v\| + \frac{\tau}{2}\|A_1(t)v\|$.

3.2. Stability

First of all, we define the operators $-A_0(t) = -A(t)|_{\mathrm{Ker}\, B}$, which are assumed to be maximal and monotone in $\mathscr{H}$, i.e.

$$\begin{cases} \forall\, h(t) \in \mathscr{H},\ \exists u(t) \in \mathscr{D} \cap \mathrm{Ker}\, B \text{ such that } u(t) - A_0(t)u(t) = h(t), & \text{and} \\ \langle -A_0(t)v, v\rangle \geqslant 0, \quad \forall v \in \mathscr{D} \cap \mathrm{Ker}\, B, \end{cases}$$

and, in a similar way, we define $-A_{i,0}(t) = -A_i(t)|_{\mathrm{Ker}\, B_i}$ and we assume that the chosen splitting makes that $-A_{i,0}(t)$ preserve the properties of maximality and monotonicity of $-A_0(t)$.

Using a classical definition of stability, we say that our method (7) is stable if the difference between the solution $(u_n : n = 0, 1, \ldots, n_f)$ of (7) and the solution $(v_n : n = 0, 1, \ldots, n_f)$ of the perturbed scheme

$$\begin{cases} \begin{cases} V_n^j = V_n^{j-1} + \tau \sum_{k=j-1}^{j} d_k (A_{i_k}(t_{n,k}) V_n^k + f_{i_k}(t_{n,k})) + \delta_n^j, \\ B_{i_j} V_n^j = g(t_{n,j}) \qquad j = 2, 3, \ldots, 2m-1, \ \text{with } V_n^1 = v_n, \end{cases} \\ v_{n+1} = V_n^{2m-1}, \ n = 0, 1, \ldots, n_f - 1, \end{cases}$$

where $v_0 = u_0 + \delta_0$ satisfies the following bound in suitable norms $\|\cdot\|_{\bullet,i}$:

$$\|v_{n+1} - u_{n+1}\|_{\bullet,n+1} \leqslant C \left(\|\delta_0\|_{\bullet,0} + \sum_{i=0}^{n} \sum_{j=2}^{2m-1} \|\delta_i^j\| \right) \quad \forall\, n = 0, 1, \ldots, n_f - 1. \tag{10}$$

It is not difficult to notice that the difference between the original solution of (7) and the perturbed solution satisfies the recurrence

$$v_{n+1} - u_{n+1} = R_n(v_n - u_n) + \sum_{j=2}^{2m-1} S_{j,n}\delta_n^j,$$

where $R_n \equiv (\mathscr{I} - (\tau/2)A_{1,0}(t_{n,2m-1}))^{-1} T_{2m-2,n} T_{2m-3,n} \cdots T_{2,n}\ (\mathscr{I} + (\tau/2)A_{1,0}(t_{n,1}))$, $S_{j,n} \equiv (\mathscr{I} - (\tau/2)A_{1,0}(t_{n,2m-1}))^{-1} T_{2m-2,n} T_{2m-3,n} \cdots T_{j,n}$, for $j = 2, \ldots, 2m-2$, and $S_{2m-1,n} \equiv (\mathscr{I} - (\tau/2)A_{1,0}(t_{n,2m-1}))^{-1}$, being $T_{k,n} = (\mathscr{I} + \tau d_k A_{i_k,0}(t_{n,k}))(\mathscr{I} - \tau d_k A_{i_k,0}(t_{n,k}))^{-1}$. Consequently

$$v_{n+1} - u_{n+1} = R_n R_{n-1} \cdots R_0 \delta_0 + \sum_{k=0}^{n} \sum_{j=2}^{2m-1} R_n R_{n-1} \cdots R_{n-k+1} S_{j,n-k} \delta_{n-k}^j.$$

In the case of considering operators $\{A_i(t)\}_{i=1}^m$ which commute and satisfy $\|A_i(t')v - A_i(t)v\| \leqslant |t - t'|\, M_i \|A_i(t)v\|,\ \forall t, t' \in [t_0, T],\ \forall v \in \mathscr{D}_i$, we can use certain results from [3] to prove $\|R_n\| \leqslant (1 + C\tau)$ and $\|S_{j,n}\| \leqslant 1,\ \forall j = 2, 3, \ldots, 2m-1$; from these bounds, the stability result (10) is immediately deduced in the norm $\|\cdot\|$.

In the case of considering a splitting in operators which do not necessarily commute, we have proven the following bounds for any $k \in \{0, \ldots, n\}$ $\|R_n R_{n-1} \cdots R_{n-k} v\|_{1,t_{n+1}} \leqslant C\|v\|_{1,t_{n-k}}$, $\|R_n R_{n-1} \cdots R_{n-k+1} S_{j,n-k} v\|_{1,t_{n+1}} \leqslant C\|v\|\ \forall j = 2, \ldots, 2m-1$; from these results we can also deduce the stability property (10) in the norms $\|\cdot\|_{1,t_i}$. Finally, combining in a classical way this stability property with the consistency of order $\overline{q}[l]$ it is easy to deduce the convergence of order $\overline{q}[l]$ of semidiscrete scheme (7), i.e., $\|u(t_n) - u_n\|_{1,t_n} \leqslant C\tau^{\overline{q}[l]},\ n = 1, 2, \ldots, n_f$ ($\|u(t_n) - u_n\| \leqslant C\tau^{\overline{q}[l]}$ for the commutative case).

3.3. Spatial discretization and convergence of the numerical algorithm

Applying a standard spatial discretization procedure to the stationary problems which arise in each internal stage of (7) we obtain the numerical algorithm

$$\begin{cases} \begin{cases} U_{n,h}^j = u_{n,h} + \tau \sum_{k=1}^{j} a_{jk}^{i_k} (A_{i_k h}(t_{n,k})\, U_{n,h}^k + f_{i_k h}(t_{n,k})), \\ B_{i_j h} U_{n,h}^j = g_h(t_{n,j}), \qquad\qquad j = 1, \ldots, s, \end{cases} \\ u_{n+1,h} = u_{n,h} + \tau \sum_{j=1}^{s} b_j^{i_j} (A_{i_j h}(t_{n,j})\, U_{n,h}^j + f_{i_j h}(t_{n,j})), \quad n = 0, 1, \ldots, n_f - 1. \end{cases} \tag{11}$$

For each $i \in \{1, \ldots, m\}$, $A_{i,h}(t)$ and $B_{i,h}$ are linear operators, defined on suitable finite-dimensional Hilbert spaces $(\mathscr{H}_h, \|.\|_h)$ and $(\mathscr{H}_h^b, \|.\|_h^b)$, which are assumed to be consistent approximations of order r of $A_i(t)$ and B_i, respectively. It is also assumed that operators $-A_{i,h}(t)$ preserve the maximality and monotonicity properties of $-A_i(t)$. Besides, $f_{i,h}(t)$, $g_h(t)$ and $r_h(t)u(t)$ denote certain restrictions or projections of $f_i(t)$, $g(t)$ and $u(t)$, respectively.

Under the previous hypotheses, the following unconditional convergence result can be deduced for (11) (see [10]) $\|E_{\tau,h}^{[l]}\|_{1,t_n,h} \leqslant C(h^r + \tau^{\overline{q}[l]})$, where $E_{\tau,h}^{[l]} \equiv r_h(t_n)u(t_n) - u_{n,h}^{[l]}$ is the global error obtained with (11) considering l improvements for the boundary conditions imposed to the internal stages. Therefore, we obtain for our proposal an unconditional convergence result of order r in space and order $\overline{q}[l] = 0, 1$

or 2 in time, depending on the boundary conditions of problem (1) and the improvements carried out for the boundary conditions considered for the internal stages of the method.

4. Numerical examples

4.1. A 3D diffusion-reaction problem: alternating direction technique

We face here the numerical resolution of the following evolutionary problem

$$\begin{cases} \dfrac{\partial u}{\partial t} = (1+\mathrm{e}^{-t}xyz)\Delta u - 2xyzu + f, \quad (t,x,y,z) \in (0,2)\times\Omega, \\ u(0,x,y,z) = \cos(\pi x)\cos(\pi y)\cos(\pi z), \quad (x,y,z)\in\Omega, \\ u(t,x,y,z) = g(t,x,y,z), \quad (t,x,y,z)\in[0,2)\times\partial\Omega, \end{cases} \tag{12}$$

where $\Omega = (0,1)^3 \subseteq \mathbb{R}^3$; the source term f and the time-dependent boundary data g have been chosen such that $u(t,x,y,z) = \mathrm{e}^{-t}\cos(\pi x)\cos(\pi y)\cos(\pi z)$ is the exact solution of (12). For this example we have combined our method with $m = 3$ and the following alternating direction type splitting: $A_1(t) = (1+\mathrm{e}^{-t}xyz)(\partial^2 u/\partial x^2) - \frac{2}{3}xyzu$, $A_2(t) = (1+\mathrm{e}^{-t}xyz)(\partial^2 u/\partial y^2) - \frac{2}{3}xyzu$, $A_3(t) = (1+\mathrm{e}^{-t}xyz)(\partial^2 u/\partial z^2) - \frac{2}{3}xyzu$ and $f_i = \frac{1}{3}f$, $i = 1,2,3$, with a central spatial discretization.

The maximum global errors have been computed as follows:

$$E^{[l]}_{\tau,h} = \max_{n,i,j,k} |u(t_n,x_i,y_j,z_k) - u^{[l]}_{n,i,j,k}|, \quad (t_n = n\tau, x_i = ih,\ y_j = jh,\ z_k = kh),$$

where $u^{[l]}_{n,i,j,k}$ is the numerical solution obtained with our totally discrete scheme (11) considering for the internal stages boundary data which have been improved l times. From these quantities we have computed the numerical orders of convergence $o^{[l]}_{\tau,h} = \log(E^{[l]}_{\tau,h}/E^{[l]}_{\tau/2,h/2})/\log 2$. We show in each cell of Table 1 the global errors (upper numbers) and the numerical orders of convergence (lower ones) computed for different time steps and spatial mesh sizes satisfying $N\tau = 0.8$, where $N = 1/h$. We observe that order 0 appears in the case of considering classical boundary values for the internal stages ($l = 0$) and that this order is increased until 2, avoiding completely the order reduction phenomenon, if we use the modifications explained before.

Table 1
Global errors and convergence orders for example 1

	$N=8$	$N=16$	$N=32$	$N=64$	$N=128$	$N=256$
$l=0$	7.502E − 3	5.763E − 3	5.164E − 3	5.081E − 3	5.081E − 3	5.082E − 3
	0.38049	0.15827	0.02344	0.00000	−0.00039	
$l=1$	2.903E − 3	1.304E − 3	5.596E − 4	2.261E − 4	8.200E − 5	2.689E − 5
	1.15427	1.22094	1.30709	1.46349	1.60865	
$l=2$	1.936E − 3	6.170E − 4	1.831E − 4	4.887E − 5	1.239E − 5	3.113E − 6
	1.64975	1.75244	1.90582	1.97950	1.99295	

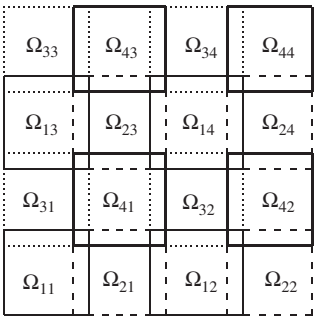

Fig. 1. Domain decomposition considered.

4.2. Domain decomposition of a 2D convection-diffusion-reaction problem

We consider here the following problem:

$$\begin{cases} \dfrac{\partial u}{\partial t} = (1+\mathrm{e}^{-t})\Delta u + \left(y-\dfrac{1}{2}\right)\dfrac{\partial u}{\partial x} - \left(x-\dfrac{1}{2}\right)\dfrac{\partial u}{\partial y} - (1+2xy)\mathrm{e}^{-2t}u, \\ \qquad\qquad (t,x,y)\in(0,2)\times\Omega, \\ u(0,x,y) = \mathrm{e}^{9+(1/((x-1/2)^2+(y-1/2)^2-1/9))} \quad (x,y)\in\Omega, \\ u(t,x,y) = 0, \quad (t,x,y)\in[0,2)\times\partial\Omega. \end{cases} \tag{13}$$

and a splitting in four terms related to a decomposition of the square $\Omega=(0,1)^2\subseteq\mathbb{R}^2$ as the union of four overlapped subdomains, each one of them consisting of four disjoint connected components: $\Omega=\bigcup_{i=1}^4\Omega_i$, where $\Omega_i=\bigcup_{j=1}^4\Omega_{ij}$ with $\Omega_{ij}\cap\Omega_{ik}=\emptyset$ if $j\neq k$, see Fig. 1.

Now we must construct a smooth partition of unity subordinated to this domain decomposition; it will consist of four functions $\{\psi_i\}_{i=1}^4$. Each one of these functions is associated with one subdomain in such a way that ψ_i takes the value 1 in the points that belong to Ω_i and not to any other subdomain, takes the value 0 in the points that do not belong to Ω_i and varies smoothly from 1 to 0 in the overlaps of Ω_i with the rest of subdomains.

To specify the smooth partition of unity chosen for this example, we define

$$i_1(x) = \begin{cases} 1 & \text{if } x\in\left[0,\dfrac{1}{4}-d\right]\cup\left[\dfrac{1}{2}+d,\dfrac{3}{4}-d\right], \\ 0 & \text{if } x\in\left[\dfrac{1}{4}+d,\dfrac{1}{2}-d\right]\cup\left[\dfrac{3}{4}+d,1\right], \\ \dfrac{1}{2}+(-1)^{4\alpha}\left(\dfrac{3}{4d}(x-\alpha)-\dfrac{1}{4d^3}(x-\alpha)^3\right) & \text{if } x\in[\alpha-d,\alpha+d],\ \alpha=\dfrac{1}{4},\dfrac{1}{2},\dfrac{3}{4} \end{cases}$$

and $i_2(x)=1-i_1(x)$, where the chosen size for the overlapping zones is $d=\frac{1}{8}$. We define the following partition of unity in Ω: $\psi_1(x,y)=i_1(x)i_1(y)$, $\psi_2(x,y)=i_2(x)i_1(y)$, $\psi_3(x,y)=i_1(x)i_2(y)$ and $\psi_4(x,y)=i_2(x)i_2(y)$. Using this partition we have made the following splittings: $A_i(t)=\psi_i A(t)$, $f_i=\psi_i f$,

Table 2
Global errors and convergence orders for example 2

$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$
1.166E − 1	5.013E − 2	2.064E − 2	6.893E − 3	1.652E − 3	4.236E − 4	1.022E − 4
1.21729	1.28022	1.58222	2.06080	1.96347	2.05182	

$i = 1, 2, 3, 4$. We have obtained again a totally discrete scheme applying our method (with $m = 4$ levels and six implicit internal stages) as time integrator combined with classical central differences for the spatial discretization.

It is interesting to notice that for each internal stage we have to solve a linear system in just the mesh points of one of the subdomains and not in the whole spatial domain Ω. Moreover, the fact that each subdomain consists of four disjoint components offers us the possibility to parallelize the needed calculations since the system involved in each internal stage can be reduced to four uncoupled linear systems of smaller dimensions. This is the typical improvement that the use of the classical domain decomposition technique provides. Note also that our method has got an additional advantage with respect to classical domain decomposition techniques because we do not have additional cost due to processes of type Schwarz iterations.

As we do not know the exact solution of problem (13), we have used the double mesh principle to estimate the global errors, i.e., $E^{[0]}_{\tau,h} \approx \max_{n,i,j} |u^{\tau}_{n,h}(i, j) - u^{\tau/2}_{n,h/2}(i, j)|$, where $u^{\tau}_{n,h}$ is the numerical solution obtained considering time step τ and mesh size h and $u^{\tau/2}_{n,h/2}$ is the numerical solution obtained after two steps of size $\tau/2$ in a mesh whose size is $h/2$; we compare both numerical solutions in the points of the coarser grid. Notice also that in this problem we have homogeneous boundary conditions and that is the reason why we can achieve order 2 considering the classical boundary conditions for the internal stages. Both global errors and estimated numerical orders of convergence obtained for different time steps τ satisfying $N\tau = 0.32$ are shown in Table 2.

For the two examples contained in this section we have performed the same type of experiments substituting our method by a two-cycle alternating direction method with the corresponding number of levels. We have used the same time step sizes τ and numbers of mesh points N. We have also used improved boundary conditions for the first example. For these experiments the maximum global errors have been 40% larger, in average, than the errors provided by our method. Besides, we want to remark that in the first example the two-cycle method (six implicit stages) has a 50% extra computational cost per time step compared to our method (four implicit stages). In the second example, the computational cost of the two-cycle method (eight implicit stages) is 33% larger than the required one by our method (six implicit stages).

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