

AVOIDING THE ORDER REDUCTION OF RUNGE-KUTTA METHODS FOR LINEAR INITIAL BOUNDARY VALUE PROBLEMS

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ABSTRACT. A new strategy to avoid the order reduction of Runge-Kutta methods when integrating linear, autonomous, nonhomogeneous initial boundary value problems is presented. The solution is decomposed into two parts. One of them can be computed directly in terms of the data and the other satisfies an initial value problem without any order reduction. A numerical illustration is given. This idea applies to practical problems, where spatial discretization is also required, leading to the full order both in space and time.

1. INTRODUCTION

Let us consider an abstract initial value problem (IVP)

$$(1.1) \quad \begin{cases} u'(t) = Au(t) + f(t), & 0 \leq t \leq T, \\ u(0) = u_0, \end{cases}$$

where $A : D(A) \subset X \rightarrow X$ is the infinitesimal generator of a C_0 -semigroup in a Banach space X , $f : [0, T] \rightarrow X$ and $u_0 \in X$. It is well known that many evolutionary problems of practical interest, either hyperbolic or parabolic, can be written in this form [28].

Problem (1.1) is integrated in time by using a Runge-Kutta (RK) method with Butcher array

$$(1.2) \quad \begin{array}{c|c} \mathbf{c} & \mathcal{A} \\ \hline & \mathbf{b}^T \end{array},$$

with $\mathbf{c} = (c_i)_{i=1}^s \in \mathbb{R}^s$, $\mathbf{b} = (b_i)_{i=1}^s \in \mathbb{R}^s$, $\mathcal{A} = (a_{ij})_{i,j=1}^s \in \mathbb{R}^{s \times s}$. Given an approximation $u_n \in X$ to $u(t_n)$, $0 \leq t_n < T$, the numerical approximation u_{n+1} to $u(t_{n+1})$ at $t_{n+1} = t_n + k_n \leq T$ is defined by

$$(1.3) \quad u_{n+1} = u_n + k_n(\mathbf{b}^T \otimes A)U_n + k_n(\mathbf{b}^T \otimes I)F(t_n),$$

where $F(t_n) = (f(t_n + k_n c_i))_{i=1}^s$ and $U_n \in X^s$ is the solution of

$$(1.4) \quad U_n = \mathbf{e} \otimes u_n + k_n(\mathcal{A} \otimes A)U_n + k_n(\mathcal{A} \otimes I)F(t_n),$$

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with $\mathbf{e} = [1, \dots, 1]^T \in \mathbb{R}^s$. Here, and throughout the paper, I stands for the identity operator in any space. It is known that for sufficiently small step-sizes k_n , (1.4) possesses a unique solution [5]. Let $u \in C^{p+1}([0, T], X)$ be a solution of (1.1), p being the classical order of the method. Under natural stability requirements, for fixed step-sizes $k_n = k$ and homogeneous problems (i.e., $f = 0$), the error $\|u(t_n) - u_n\|$ behaves like $O(k^p)$ [11]. However, for nonhomogeneous problems and unbounded operators A , it turns out that the classical order p is not attained [10, 24, 32]. This is the so-called order reduction phenomenon. In fact, for nonhomogeneous problems the order of convergence is rather governed by the stage order q of the method. Set

$$\mathbf{w}_l = \mathbf{c}^l - lAc^{l-1}, \quad 1 \leq l \leq p,$$

where $\mathbf{c}^l = (c_i^l)_{i=1}^s$ and $\mathbf{c}^0 = \mathbf{e}$. Recall that q is defined as the largest integer for which $\mathbf{w}_l = 0$, $1 \leq l \leq q$. Typically the order of convergence is $\min\{p, q + 1 + \theta\}$ with $0 \leq \theta < 2$ (possibly θ is not integer) [24]. Let us point out that, in the context of PDEs, this order reduction does not occur in the interior of the spatial domain [21].

IVPs of the form (1.1) are a particular instance of the more general initial boundary value problems (IBVPs)

$$(1.5) \quad \begin{cases} u'(t) = \tilde{A}u(t) + f(t), & 0 \leq t \leq T, \\ u(0) = u_0, \\ \partial u(t) = g(t), & 0 \leq t \leq T, \end{cases}$$

where $\tilde{A} : D(\tilde{A}) \subset X \rightarrow X$ is a linear extension of A , ∂ is a linear mapping from $D(\tilde{A})$ to another Banach space Y and $g : [0, T] \rightarrow Y$. The precise conditions to be fulfilled by these operators are described in Section 2 (see also [5]). Notice that the IVPs (1.1) arising in the applications always correspond to certain natural IBVPs (1.5) with $g = 0$. When (1.5) is integrated in time with the RK method (1.2), the order of convergence is $\min\{p, q + \theta\}$ with $0 \leq \theta < 2$ [5]. Thus, for IBVPs the order reduction is more severe than for IVPs.

Different remedies have been proposed in the literature to avoid the order reduction [1, 2, 3, 5, 12, 19, 20, 30, 32]. In the present paper a new strategy yielding the full order p in the time integration of (1.5) is introduced. This strategy cannot be applied directly to the IVP (1.1). However, this is not a serious drawback since in practice, as we mentioned above, (1.1) can be written in the format (1.5).

The basic idea is as follows. The solution of (1.5) is decomposed as $u(t) = v(t) + u^*(t)$, where $v(t)$ can be computed directly in terms of the data and $u^*(t)$ is the solution of a suitable IVP of the form (1.1). The key point of this construction is that $u^*(t) \in D(A^{p-q})$, so that there is no order reduction in the RK approximation to $u^*(t)$. This strategy is studied in Section 3. Since the implementation of our strategy demands the solution of additional stationary problems at each step (see Remark 3.6 below), a high cost may result. Thus, though the strategy is interesting from a theoretical point of view, the standard implementation of an RK method with appropriate stage order could be advantageous in some instances. Numerical experiments are presented in Section 4, illustrating the theoretical results. In the final Section 5 it is shown that the remedy proposed in the present paper can also be accommodated in practical situations, where full discretizations of (1.5) are

required. It is worth mentioning here that, as different from previous approaches [2, 3], standard spatial discretizations can be used.

2. ABSTRACT INITIAL BOUNDARY VALUE PROBLEMS

In this section we describe briefly the setting of [28]. Let X, Y be two Banach spaces. The norms in X and Y and the operator norms are denoted by $\|\cdot\|$. Let $\tilde{A} : D(\tilde{A}) \subset X \rightarrow X, \partial : D(\tilde{A}) \subset X \rightarrow Y$ be linear operators. We assume that

H1. The operator $(\tilde{A}, \partial) : D(\tilde{A}) \subset X \rightarrow X \times Y$ is closed. Moreover, $\partial : D(\tilde{A}) \subset X \rightarrow Y$ is onto.

H2. Set $D(A) = \ker(\partial) = \{x \in D(\tilde{A}) / \partial x = 0\}$. Then the restriction $A = \tilde{A}|_{D(A)} : D(A) \subset X \rightarrow X$ is the infinitesimal generator of a C_0 -semigroup $S(t), t \geq 0$, in X .

It is well known that there exist $M > 0$ and $\omega \in \mathbb{R}$ such that $\|S(t)\| \leq Me^{\omega t}, t \geq 0$ (see, e.g., [31]).

In [28] it is proved that **H1–H2** imply the following condition: For each $\lambda > \omega$ there exists a linear and bounded operator $K(\lambda) : Y \rightarrow X$ such that, for each $y \in Y, x = K(\lambda)y \in X$ is the unique solution of the problem

$$(2.1) \quad \begin{cases} (\tilde{A} - \lambda)x = 0, \\ \partial x = y. \end{cases}$$

Let us denote, for an integer $r \geq 0, \tilde{W}_r = D(\tilde{A}^r)$ and $W_r = D(A^r)$. It turns out that for each $\lambda > \omega$ the operator $K(\lambda)\partial : \tilde{W}_r \rightarrow \tilde{W}_r$ is bounded, where \tilde{W}_r is endowed with the norm

$$\|x\|_{\tilde{W}_r} = \|x\| + \|\tilde{A}x\| + \dots + \|\tilde{A}^r x\|, \quad x \in \tilde{W}_r,$$

which is equivalent to the graph-norm of \tilde{A}^r .

Let $T > 0$ and let $f : [0, T] \rightarrow X$ be continuous and $g : [0, T] \rightarrow Y$ a C^1 -mapping. Assume that $u_0 \in \tilde{W}_1$ satisfies $\partial u_0 = g(0)$. Then the IBVP (1.5) has got a unique solution $u : [0, T] \rightarrow X$ [28].

Next we give an example to illustrate these concepts (see [4, 28] for additional examples).

Example 2.1. Let us consider the initial boundary value problem for the one-dimensional heat equation

$$(2.2) \quad \begin{cases} u_t(x, t) = u_{xx}(x, t) + f(x, t), & x \in [0, 1], \quad 0 \leq t \leq T, \\ u(x, 0) = u_0(x), & x \in [0, 1], \\ u(0, t) = g_0(t), & 0 \leq t \leq T, \\ u(1, t) = g_1(t), & 0 \leq t \leq T, \end{cases}$$

where $f : [0, 1] \times [0, T] \rightarrow \mathbb{R}, u_0 : [0, 1] \rightarrow \mathbb{R}, g_0, g_1 : [0, T] \rightarrow \mathbb{R}$ are given functions.

Problem (2.2) can be written in the abstract form (1.5) as follows: $X = L^p([0, 1]), 1 \leq p < +\infty$, or $X = C_0([0, 1])$ if $p = +\infty, Y = \mathbb{R} \times \mathbb{R}, D(\tilde{A}) = W^{2,p}([0, 1]) = \{\varphi \in X / \varphi'' \in X\}, \tilde{A}\varphi = \varphi''$ and $\partial\varphi = [\varphi(0), \varphi(1)]^T, \varphi \in D(\tilde{A})$. In this example $D(A) = W^{2,p}([0, 1]) \cap W_0^{1,p}([0, 1]) = \{\varphi \in W^{2,p}([0, 1]) / \varphi(0) = \varphi(1) = 0\}$ and for $\xi = [\xi_0, \xi_1]^T \in Y, K(0)\xi$ is the mapping sending $x \in [0, 1]$ to $(1-x)\xi_0 + x\xi_1$. Finally, for $r \geq 1, \tilde{W}_r = W^{2r,p}([0, 1])$ and $W_r = \{\varphi \in W^{2r,p}([0, 1]) / \varphi^{(2j)}(0) = \varphi^{(2j)}(1) = 0, 0 \leq j \leq r\}$.

Assume that $g \in C^m([0, T], Y)$ and $f^{(j)} \in C^{m-j-1}([0, T], \widetilde{W}_{m-j-1})$, $0 \leq j \leq m-1$, for some $m \geq 1$. Notice that in practice this is a natural requirement since these conditions only demand regularity of $f^{(j)}$ but they do not impose any restriction on the values of $f^{(j)}$ at the boundary of the spatial domain. This is opposite to the unnatural assumptions $f^{(j)}(t) \in W_{m-j-1}$, $0 \leq j \leq m-1$, $0 \leq t \leq T$ (see example above). Under certain compatibility conditions among the data f , g and u_0 (see [2]) the solution $u : [0, T] \rightarrow X$ of (1.5) belongs to $C^m([0, T], X) \cap C([0, T], \widetilde{W}_1)$.

As long as **H1** is satisfied, we can differentiate in equation (1.5) and get that $u'(t) \in \widetilde{W}_1$ and

$$\begin{cases} u''(t) = \widetilde{A}u'(t) + f'(t), & 0 \leq t \leq T, \\ \partial u'(t) = g'(t), & 0 \leq t \leq T. \end{cases}$$

Moreover, since $u'(t) = \widetilde{A}u(t) + f(t)$ and $f(t) \in \widetilde{W}_1$, we have $u(t) \in \widetilde{W}_2$ and then

$$u''(t) = \widetilde{A}^2u(t) + \widetilde{A}f(t) + f'(t).$$

In fact, by induction, it is easy to prove that, for $1 \leq l \leq m$ and $0 \leq t \leq T$, $u(t) \in \widetilde{W}_l$, $u^{(l-1)}(t) \in \widetilde{W}_1$ and

$$(2.3) \quad \begin{cases} u^{(l)}(t) = \widetilde{A}^l u(t) + \sum_{j=0}^{l-1} \widetilde{A}^{l-j-1} f^{(j)}(t), \\ \partial u^{(l)}(t) = g^{(l)}(t). \end{cases}$$

This also yields

$$\widetilde{A}^l u(t) = u^{(l)}(t) - \sum_{j=0}^{l-1} \widetilde{A}^{l-j-1} f^{(j)}(t),$$

so that

$$(2.4) \quad \partial \widetilde{A}^l u(t) = g^{(l)}(t) - \sum_{j=0}^{l-1} \partial \widetilde{A}^{l-j-1} f^{(j)}(t).$$

In summary, we have shown the way to obtain the boundary values of $\widetilde{A}^l u$ in terms of the data f and g and their derivatives.

In the next section we will use the related expression for $\lambda > \omega$

$$(2.5) \quad \partial(\lambda - \widetilde{A})^l u(t) = \lambda^l g(t) + \sum_{j=1}^l \binom{l}{j} \lambda^{l-j} (-1)^j \left[g^{(j)}(t) - \sum_{i=0}^{j-1} \partial \widetilde{A}^{j-i-1} f^{(i)}(t) \right],$$

which is a direct consequence of (2.4).

3. THE MAIN RESULT

Let $u : [0, T] \rightarrow X$ be a solution of (1.5). We try to write $u = v + u^*$, where $u^* : [0, T] \rightarrow X$ is the solution of a suitable IVP

$$(3.1) \quad \begin{cases} u^{*'}(t) = Au^*(t) + f^*(t), \\ u^*(0) = u_0^*, \end{cases}$$

and where $v : [0, T] \rightarrow X$, u_0^* and $f^* : [0, T] \rightarrow X$ can be computed from the data u_0, f and g in such a way that the RK method applied to (3.1) does not suffer from order reduction.

This idea is frequently used with $v(t) = Eg(t)$, where $E : Y \rightarrow X$ is a linear operator such that $\partial E y = y$ for $y \in Y$. This choice leads to the initial value problem

$$(3.2) \quad \begin{cases} u^{*'}(t) = Au^*(t) + f(t) - Eg'(t) + \tilde{A}Eg(t), \\ u^*(0) = u_0 - Eg(0). \end{cases}$$

Since $u^* \in D(A)$, then the order of the RK discretization of (3.2) is k^{q+1} (see [5, 24]). Thus, for $q < p - 1$ and this choice of v , the order reduction still appears for u^* .

Our goal is to construct a more appropriate correcting term v . To this end we define the operators $C_r(\lambda) : \tilde{W}_r \rightarrow X$ as

$$(3.3) \quad C_r(\lambda) = \sum_{s=0}^{r-1} (\lambda - A)^{-s} K(\lambda) \partial(\lambda - \tilde{A})^s, \quad \lambda > \omega, \quad r \geq 1.$$

Before defining v we give the following technical lemma which will be used in the proof of Theorem 1.

Lemma 3.1. *Let $r \geq 1, \lambda > \omega$. Then*

- (i) $C_r(\lambda)$ is a bounded operator from \tilde{W}_r to \tilde{W}_r .
- (ii) For $0 \leq j \leq r - 1$ and $x \in \tilde{W}_r$ it holds that

$$\partial(\lambda - \tilde{A})^j C_r(\lambda)x = \partial(\lambda - \tilde{A})^j x.$$

Proof. Since $K(\lambda)\partial$ is a bounded operator from \tilde{W}_{r-s} to $\tilde{W}_{r-s}, 0 \leq s \leq r - 1$, it is clear that $(\lambda - A)^{-s} K(\lambda) \partial(\lambda - \tilde{A})^s$ is a bounded operator from \tilde{W}_r to \tilde{W}_r . This proves (i).

Let $x \in \tilde{W}_1$. Since $(\lambda - \tilde{A})K(\lambda)\partial x = 0$ and $(\lambda - \tilde{A})(\lambda - A)^{-1}x = x$, it turns out that, for $x \in \tilde{W}_r, r \geq 2$,

$$(3.4) \quad \begin{aligned} (\lambda - \tilde{A})C_r(\lambda)x &= (\lambda - \tilde{A})K(\lambda)\partial x + \sum_{s=1}^{r-1} (\lambda - \tilde{A})(\lambda - A)^{-s} K(\lambda) \partial(\lambda - \tilde{A})^s x \\ &= C_{r-1}(\lambda)(\lambda - \tilde{A})x. \end{aligned}$$

We now proceed by induction in the proof of (ii). For $x \in \tilde{W}_1$,

$$C_1(\lambda)x = K(\lambda)\partial x$$

and (ii) for $r = 1$ is a direct consequence of the definition of $K(\lambda)$. Let us now assume that (ii) holds for $r - 1, r \geq 2$. Let $x \in \tilde{W}_r$. By (3.4), for $1 \leq j \leq r - 1$

$$\partial(\lambda - \tilde{A})^j C_r(\lambda)x = \partial(\lambda - \tilde{A})^{j-1} C_{r-1}(\lambda)(\lambda - \tilde{A})x.$$

Then using (ii) with $r - 1$, we conclude that

$$\partial(\lambda - \tilde{A})^j C_r(\lambda)x = \partial(\lambda - \tilde{A})^{j-1} (\lambda - \tilde{A})x = \partial(\lambda - \tilde{A})^j x.$$

Moreover, (ii) is clear for $j = 0$ since $\partial(\lambda - A)^{-1} = 0$. □

We are now in a position to define the correcting term. Assume that the solution u of (1.5) belongs to $C^{p+1}([0, T], \tilde{W}_r)$ for some $1 \leq r \leq p - q$. We want to stress

again that, in practice, this condition is natural, since it only demands the solution be smooth both in time and space. We define

$$(3.5) \quad v(t) = C_r(\lambda)u(t), \quad 0 \leq t \leq T,$$

where $C_r(\lambda)$ is given by (3.3) with $\lambda > \omega$ fixed. Observe that $r = 1$ corresponds to the usual correction mentioned above with $E = K(0)$.

Notice that, due to (2.5), $v(t)$ can certainly be computed in terms of f and g and their derivatives. For this choice of v it turns out that

$$\begin{aligned} f^*(t) &= f(t) - C_r(\lambda)u'(t) + \tilde{A}C_r(\lambda)u(t), \\ u_0^* &= [I - C_r(\lambda)]u_0. \end{aligned}$$

Assume also that $f \in C^p([0, T], X)$, $g \in C^{p+1}([0, T], Y)$. Taking derivatives in equation (1.5) and using **H1** as in Section 2 prove that $f^{(j)}(t) \in \widetilde{W}_{r-j-1}$, $0 \leq j \leq r - 1$, $0 \leq t \leq T$ and then $f^*(t)$ can again be computed in terms of the data and their derivatives. More precisely,

$$f^*(t) = [I - C_r(\lambda)]f(t) + (\lambda - A)^{-(r-1)}K(\lambda)\partial(\lambda - \tilde{A})^r u(t),$$

where $\partial(\lambda - \tilde{A})^r u(t)$ is given by (2.5). If $\omega < 0$, we can choose $\lambda = 0$ and the simpler expression

$$f^*(t) = [I - C_r(0)]f(t) - A^{-(r-1)}K(0) \left[g^{(r)}(t) - \sum_{j=0}^{r-1} \partial \tilde{A}^{r-j-1} f^{(j)}(t) \right]$$

results.

Recall that the stability function $r(z)$ of the RK method is defined by $r(z) = 1 + z\mathbf{b}^T(I - z\mathcal{A})^{-1}\mathbf{e}$. Hereafter, we suppose that there exists $\bar{k} > 0$ such that, for $0 < k \leq \bar{k}$, the operator $I - \mathcal{A} \otimes kA : D(A)^s \subset X^s \rightarrow X^s$ is invertible (see, e.g., [5]). Therefore, for $0 < k \leq \bar{k}$ the equations defining the RK approximations are solvable and the operator $r(kA)$ is well defined in X .

In the following theorem we assume that $\max k_m \leq \bar{k}$. Let us denote by u_n^* the RK approximation to the solution of (3.1) at time level t_n , $0 \leq n \leq N$. Thus, we adopt $u_n = u_n^* + v(t_n)$ as the numerical approximation to $u(t_n)$.

Theorem 3.2. *Let $u \in C^{p+1}([0, T], \widetilde{W}_r)$, $r = p - q$, be the solution of the IBVP (1.5). Assume also that $f \in C^p([0, T], X)$ and $g \in C^{p+1}([0, T], Y)$. Let $v : [0, T] \rightarrow X$ be the correcting term defined in (3.5). Then*

$$\|u(t_n) - u_n\| = \|u^*(t_n) - u_n^*\| \leq C\rho_n \sum_{m=1}^n k_{m-1}^{p+1} I_m(u),$$

where $C > 0$ is a constant and

$$\begin{aligned} \rho_n &= \left\| \prod_{m=1}^n r(k_{m-1}A) \right\|, \\ I_m(u) &= \sup_{q+1 \leq l \leq p+1} \|u^{(l)}\|_{L^\infty([t_{m-1}, t_m], \widetilde{W}_r)}. \end{aligned}$$

The constant C depends on T , A and the RK method but it is independent of u , f and g .

Proof. By Lemma 1, $I - C_r(\lambda) : \widetilde{W}_r \rightarrow \widetilde{W}_r$ is bounded. The norm of this operator is denoted by L .

Since $u^*(t) = [I - C_r(\lambda)]u(t)$, $0 \leq t \leq T$, then $u^* \in C^{p+1}([0, T], \widetilde{W}_r)$ and

$$\|u^{*(l)}(t)\|_{\widetilde{W}_r} \leq L\|u^{(l)}(t)\|_{\widetilde{W}_r}, \quad 0 \leq l \leq p + 1.$$

Moreover, again by Lemma 1, we have

$$\partial(\lambda - \widetilde{A})^j u^{(l)}(t) = \partial(\lambda - \widetilde{A})^j C_r(\lambda) u^{(l)}(t), \quad 0 \leq j \leq r - 1,$$

whence

$$\partial(\lambda - \widetilde{A})^j u^{*(l)}(t) = 0, \quad 0 \leq j \leq r - 1,$$

so that $u^{*(l)}(t) \in W_r$ for $0 \leq l \leq p + 1$, $0 \leq t \leq T$. Thus, $u^* \in C^{p+1}([0, T], W_r)$ and

$$(3.6) \quad \|A^j u^{*(l)}(t)\| \leq L\|u^{(l)}(t)\|_{\widetilde{W}_r}, \quad 0 \leq j \leq r, \quad 0 \leq l \leq p + 1.$$

Now, the proof is straightforward by well-known results concerning RK methods for nonhomogeneous problems [5, 10] and by using (3.6). \square

Remark 3.3. It makes sense to carry out corrections with $1 \leq r < p - q$. Then the arguments used in the proof of Theorem 1 show that

$$(3.7) \quad \|u(t_n) - u_n\| \leq C\rho_n \sum_{m=1}^n k_{m-1}^{q+r+1} I_m(u).$$

Furthermore the results in [5, 24] imply that if $r(\infty) \neq 1$ and under natural stability requirements, then for fixed step-sizes $k_m = k$

$$(3.8) \quad \|u(t_n) - u_n\| \leq C\rho_n k^{q+r+1} \sum_{m=1}^n I_m(u).$$

Thus, in this situation the full order p is achieved with $r = p - q - 1$.

Remark 3.4. Fractional orders of convergence are also possible. Let us assume that there exists $\mu \in (0, 1)$ such that $\widetilde{W}_1 \subset W_\mu$, where W_μ is $D((\omega^* - A)^\mu)$, for some $\omega^* > \omega$. Let us point out that this is the case indeed in many examples (see [4]). For instance in the example of equation (2.2), it turns out $\mu = 1/(2p)$, $1 \leq p \leq +\infty$. It is easy to prove that $I - C_r(\lambda)$ maps \widetilde{W}_{r+1} to $W_{r+\mu}$ continuously. Then, according to the results in [5], an extra order μ is present in (3.7) and (3.8).

Remark 3.5. If A is the infinitesimal generator of a C_0 -semigroup of contractions in a Hilbert space and the RK method is A-stable, then [16, 35]

$$\rho_n \leq e^{t_n \max\{0, \omega\}}.$$

For general C_0 -semigroups in Banach spaces and fixed step-sizes the bound

$$\rho_n \leq e^{t_n \max\{0, \omega\}} O(\sqrt{n})$$

is optimal [11, 14, 15] and half an order of convergence could be lost. In special situations this loss might not occur (see [11]).

On the other hand, if A is the infinitesimal generator of an analytic semigroup (see, e.g., [6, 14, 25, 26]), then

$$\rho_n \leq e^{t_n \max\{0, \omega\}} O(1).$$

This bound is valid even for variable step-sizes if $|r(\infty)| < 1$ [8, 26].

Remark 3.6. From the definition of $C_r(\lambda)$ it is clear that the computation of the initial condition u_0^* and each evaluation of f^* and the correcting term v require the solution of $2r - 1$ stationary problems as (2.1). In these stationary problems, derivatives of f and g are involved which, in the evaluation of v and f^* , may be replaced by appropriate approximations of order at least p . Notice also that the computation of $v(t)$ is only necessary at the time levels where output is required.

4. NUMERICAL ILLUSTRATION

In this section we present two simple experiments to illustrate the results in Section 3. Let us consider the IBVP for the one-dimensional heat equation (2.2) in the example, with $p = +\infty$, where f, u_0, g_0 and g_1 are chosen for $u(x, t) = \sin x/(1 + t)$ to be its exact solution. As mentioned at the beginning of Section 3, introducing the usual correcting term

$$v(t) = Eg(t) = g_0(t) + x[g_1(t) - g_0(t)],$$

and defining $u^* = u - v$, the original problem is transformed into the IBVP with homogeneous boundary conditions

$$(4.1) \quad \begin{cases} u_t^*(x, t) = u_{xx}^*(x, t) + f(x, t) - g_0'(t) - x[g_1'(t) - g_0'(t)], \\ u^*(x, 0) = u_0(x) - g_0(0) - x[g_1(0) - g_0(0)], \\ u^*(0, t) = 0, \\ u^*(1, t) = 0. \end{cases}$$

($x \in [0, 1], 0 \leq t \leq T$). For the spatial discretization of (4.1), given an integer $J \geq 2$, we define the uniform grid $x_j = jh, 1 \leq j \leq J$, in the interval $[0, 1]$, where $h = 1/(J + 1)$. The second derivative is approximated using the standard three-point finite differences.

For the time integration we use the singly diagonally implicit RK method proposed in [13] with Butcher array

$$\begin{array}{c|ccc} \gamma & & & \\ 1/2 & 1/2 - \gamma & \gamma & \\ 1 - \gamma & 2\gamma & 1 - 4\gamma & \gamma \\ \hline & \delta & 1 - 2\delta & \delta \end{array},$$

where

$$\gamma = \frac{1}{\sqrt{3}} \cos\left(\frac{\pi}{18}\right) + \frac{1}{2}, \quad \delta = \frac{1}{6(2\gamma - 1)^2}.$$

This method has order $p = 4$, stage order $q = 1$, is A -stable and $|r(\infty)| < 1$. According to the results included in [5, 24] and, since $u^* \in D(A)$ and $\mu = 0$ (see Remark 2), the expected order of the error of the time integrator is three.

In our numerical experiments, to clearly observe the error due to the time integrator, we integrate the differential system

$$(4.2) \quad \begin{cases} u_h^*(t) = A_h u_h^*(t) + \hat{f}_h^*(t), & 0 \leq t \leq T, \\ u_h^*(0) = [u^*(x_1, 0), \dots, u^*(x_J, 0)]^T, \end{cases}$$

where

$$\hat{f}_h^*(t) = (P_h A - A_h P_h)u^*(x, t) + P_h f^*(t).$$

TABLE 1. Errors for $r = 1$

$h = k$	5.000e-02	2.500e-02	1.250e-02	6.250e-03	3.125e-03
Error	5.9752e-07	7.0579e-08	8.2533e-09	9.8621e-10	1.2009e-10
Order	3.08	3.10	3.10	3.04	

TABLE 2. Errors for $r = 2$

$h = k$	5.000e-02	2.500e-02	1.250e-02	6.250e-03	3.125e-03
Error	5.5893e-08	5.5342e-09	4.6049e-10	3.4250e-11	2.3790e-12
Order	3.34	3.59	3.75	3.85	

Here for $\varphi \in D(A)$, $P_h\varphi(x, t) = [\varphi(x_1, t), \dots, \varphi(x_J, t)]^T$ and A_h is the three-point approximation to A . The exact solution of (4.2) is the restriction of the exact solution of (4.1) to the grid points, so that there is no spatial error.

In Table 1 the global errors when $h = k$ have been reported. We observe that when halving k the global errors are approximately divided by 8, as corresponding to the third order. This means that the order reduction is still present because the classical order of the RK method is four.

In our second experiment we transform the original IBVP (2.2) into the IVP (3.1) by introducing the correcting term with $r = 2$

$$v = C_2(0)u = Eg + A^{-1}E[g' - \partial f].$$

Now $u^* = u - v \in D(A^2)$ and, according to Remark 1, the global error of the time integrator should exhibit the full order four. In Table 2 the global errors for this second experiment are presented. The quantities in the last row approach the full order four as k goes to zero, as expected.

5. THE FULLY DISCRETE PROBLEM

When solving IBVPs arising in PDEs using the method of lines, first it is necessary to discretize with respect to the spatial variable and then to time integrate the resulting system of ordinary differential equations. Then, in practice, we do not time integrate the IVP (3.1) but a discrete version of it. In the numerical experiments shown in Section 4 we have computed u_0^* and f^* exactly and then we have discretized with respect to the spatial variable. However, in general, it is not possible to compute (3.1) exactly because it would require the solution of certain stationary problems which, in most cases, must be solved numerically. In this section we prove that the result in Section 3 also applies to the fully discrete problem. As we mentioned in the introduction, one advantage of our approach is that standard spatial discretizations can be used.

Let us denote by $0 < h < h_0$ the parameter of the spatial discretization and let $(X_h, \|\cdot\|)$ be a family of normed spaces approximating X [17, 29]. The link between X and X_h is given by certain linear mappings $P_h : X \rightarrow X_h$. For $x \in X$, $P_h x$ is the approximation to x in X_h . The operator $A : D(A) \rightarrow X$ is approximated by linear operators $A_h : X_h \rightarrow X_h$. As usual [17, 29], we assume that the semigroups e^{tA_h} are uniformly bounded, i.e., $\|e^{tA_h}\| \leq M e^{\omega t}$, $t \geq 0$, for some M and ω independent of h . In this situation, the consistency of the spatial discretization is measured by

$$(5.1) \quad \varphi_s(h) := \|(\omega^* - A_h)^{-1}(A_h P_h - P_h A)\|_{W_s \rightarrow X_h},$$

for some $s > 0$ and $\omega^* > \omega$. Recall that $W_s = D(A^s)$.

For instance, in the case of finite elements of degree $2s - 1$ and a second-order elliptic operator A , it turns out that $\varphi_s(h) = O(h^{2s})$ in the L_2 -norm [36]. If a finite difference scheme of order $2s - 2$ is used instead, again for an elliptic operator A of second order, we have

$$\|(A_h P_h - P_h A)\|_{W_s \rightarrow X_h} = O(h^{2s-2})$$

and, since $\|(\omega^* - A_h)^{-1}\| \leq M/(\omega^* - \omega)$, then $\varphi_s(h) = O(h^{2s-2})$.

We also assume that $\varphi_s(h)$ balances the behaviour of $\|A_h\|$ in the sense that

$$(5.2) \quad \|A_h^{m-1}(A_h P_h - P_h A)\|_{W_m \rightarrow X_h} \leq \lambda, \quad 1 \leq m \leq s,$$

for some $\lambda > 0$ independent of h . This condition is clearly satisfied in the context of either finite elements or finite differences mentioned above, where $\|A_h\| = O(h^{-2})$.

In the present context of IBVPs also the operators $C_r(\lambda)$ must be approximated. In practice, this can be done by using either boundary elements [9, 18] or finite differences [22, 23] for discretizing $K(\lambda)\partial$. Thus, we assume that $P_h f^*(t)$, $P_h v(t)$ and $P_h u_0^*$ are approximated by $f_h^*(t)$, $v_h(t)$ and $u_{h,0}^*$ in X_h . For solutions u taking values in \widetilde{W}_s we denote by $\psi_s(h)$ the error of these approximations, i.e.,

$$\begin{aligned} \|P_h f^*(t) - f_h^*(t)\| &= O(\psi_s(h)), \\ \|P_h u_0^* - u_{h,0}^*\| &= O(\psi_s(h)), \\ \|P_h v(t) - v_h(t)\| &= O(\psi_s(h)), \end{aligned}$$

as $h \rightarrow 0+$, uniformly in $0 \leq t \leq T$.

After the spatial discretization of (3.1), we have to time integrate the differential system

$$(5.3) \quad \begin{cases} u_h^{*'}(t) = A_h u_h^*(t) + f_h^*(t), \\ u_h^*(0) = u_{h,0}^*. \end{cases}$$

Let us denote by $u_{h,n}^*$ the RK approximation to the solution of (5.3) at time level $t_n = nk$. The fully discrete approximation to $u(t_n)$ is thus defined by $u_{h,n} = u_{h,n}^* + v_h(t_n)$.

The fully discrete scheme is said to be stable if there exist $\bar{k} > 0$ and $\rho = \rho(T) > 0$ such that, for $0 < k \leq \bar{k}$, the operator $I - \mathcal{A} \otimes kA_h : X_h \rightarrow X_h$ is invertible, $0 < h < h_0$, and

$$\|r(kA_h)^n\| \leq \rho, \quad 0 \leq nk \leq T.$$

Under these assumptions we can establish the result for the full discretization.

Theorem 5.1. *Let $u \in C^{p+1}([0, T], \widetilde{W}_r)$, $r = p - q$, be the solution of the IBVP (1.5). Assume also that $f \in C^p([0, T], X)$, $g \in C^{p+1}([0, T], Y)$. Assume that (5.2) is satisfied for $s = r$ and that the fully discrete scheme is stable. Then, for $0 < k \leq \bar{k}$,*

$$\|P_h u(t_n) - u_{h,n}\| \leq Ct_n[k^p + \varphi_r(h) + \psi_r(h)],$$

where $C = C(u, \lambda, \rho)$.

Proof. For simplicity in the proof we suppose $\omega < 0$.

Set $e_{h,n}^* = P_h u^*(t_n) - u_{h,n}^*$. From the definition of $u_{h,n}$ and the relation $u^*(t) = u(t) - v(t)$ it is clear that

$$\|P_h u(t_n) - u_{h,n}\| \leq \|e_{h,n}^*\| + \|P_h v(t_n) - v_h(t_n)\|.$$

The second term is bounded by $O(\psi_r(h))$ and only $e_{h,n}^*$ must be analyzed. Let $\bar{u}_{h,n+1}^*$ be the RK approximation to the solution of

$$(5.4) \quad x'_h(t) = A_h x_h(t) + f_h^*(t)$$

at t_{n+1} , starting from $x_h(t_n) = P_h u^*(t_n)$. Then,

$$e_{h,n+1}^* = (\bar{u}_{h,n+1}^* - u_{h,n+1}^*) + (P_h u^*(t_{n+1}) - \bar{u}_{h,n+1}^*).$$

The first two terms on the right-hand side are numerical solutions of (5.4) after one step with initial conditions $P_h u^*(t_n)$ and $u_{h,n}^*$ respectively, so that

$$(5.5) \quad e_{h,n+1}^* = r(kA_h)e_{h,n}^* + (P_h u^*(t_{n+1}) - \bar{u}_{h,n+1}^*).$$

Next, in order to use the variation-of-constants formula, it is sufficient to study the truncation term $P_h u^*(t_{n+1}) - \bar{u}_{h,n+1}^*$. We set $F^*(t) = (f^*(t + c_i k))_{i=1}^s$, $U^*(t) = (u^*(t + c_i k))_{i=1}^s$ and $U^{*'}(t) = (u^{*'}(t + c_i k))_{i=1}^s$ for the differential equation (3.1) and $F_h^*(t) = (f_h^*(t + c_i k))_{i=1}^s$ for (5.4).

Direct substitution of $P_h u^*$ into the equations defining the stages of the RK approximation to the solution of (5.4) defines the defects $\tau_{h,n}$ by

$$(5.6) \quad P_h U^*(t_n) = (\mathbf{e} \otimes I) P_h u^*(t_n) + (\mathcal{A} \otimes kA_h) P_h U^*(t_n) + k(\mathcal{A} \otimes I) F_h^*(t_n) + \tau_{h,n},$$

which can also be written as

$$\begin{aligned} P_h U^*(t_n) &= P_h [(\mathbf{e} \otimes I) u^*(t_n) + k\mathcal{A} \otimes U^{*'}(t_n)] \\ &+ k\mathcal{A} \otimes (A_h P_h - P_h A) U^*(t_n) + k(\mathcal{A} \otimes I) (F_h^* - P_h F^*)(t_n) + \tau_{h,n}. \end{aligned}$$

Taylor expansions of U^* and $U^{*'}$ at t_n show

$$U^*(t_n) - (\mathbf{e} \otimes I) u^*(t_n) - k\mathcal{A} \otimes U^{*'}(t_n) = \sum_{l=q+1}^p \frac{k^l}{l!} (\mathbf{w}_l \otimes I) u^{*(l)}(t_n) + O(k^{p+1})$$

(recall that $\mathbf{w}_l = \mathbf{c}^l - l\mathcal{A}\mathbf{c}^{l-1}$, for $q+1 \leq l \leq p$). Then

$$(5.7) \quad \begin{aligned} \tau_{h,n} &= \sum_{l=q+1}^p \frac{k^l}{l!} (\mathbf{w}_l \otimes I) P_h u^{*(l)}(t_n) - k\mathcal{A} \otimes (A_h P_h - P_h A) U^*(t_n) \\ &- k(\mathcal{A} \otimes I) (F_h^* - P_h F^*)(t_n) + O(k^{p+1}). \end{aligned}$$

On the other hand, the internal stages $\bar{U}_{h,n}^*$ for the RK approximation to the solution of (5.4) starting from $P_h u^*(t_n)$ satisfy

$$(5.8) \quad \bar{U}_{h,n}^* = (\mathbf{e} \otimes I) P_h u^*(t_n) + (\mathcal{A} \otimes kA_h) \bar{U}_{h,n}^* + k(\mathcal{A} \otimes I) F_h^*(t_n).$$

Subtracting (5.8) from (5.6) we get

$$P_h U^*(t_n) - \bar{U}_{h,n}^* = (\mathcal{A} \otimes kA_h) [P_h U^*(t_n) - \bar{U}_{h,n}^*] + \tau_{h,n},$$

which using (5.7) leads to

$$(5.9) \quad \begin{aligned} P_h U^*(t_n) - \bar{U}_{h,n}^* &= (I - \mathcal{A} \otimes kA_h)^{-1} \sum_{l=q+1}^p \frac{k^l}{l!} (\mathbf{w}_l \otimes I) P_h u^{*(l)}(t_n) \\ &- (I - \mathcal{A} \otimes kA_h)^{-1} k\mathcal{A} \otimes (A_h P_h - P_h A) U^*(t_n) \\ &- (I - \mathcal{A} \otimes kA_h)^{-1} k(\mathcal{A} \otimes I) (F_h^* - P_h F^*)(t_n) + O(k^{p+1}). \end{aligned}$$

Let us now consider the equation that defines the RK approximation to the solution of (5.4) at time level t_{n+1} . Direct substitution of $P_h u^*$ into this equation defines the defects $\delta_{h,n+1}$ by

$$(5.10) \quad P_h u^*(t_{n+1}) = P_h u^*(t_n) + k(\mathbf{b}^T \otimes A_h)P_h U^*(t_n) + k(\mathbf{b}^T \otimes I)F_h^*(t_n) + \delta_{h,n+1},$$

which can be written as

$$P_h u^*(t_{n+1}) = P_h [u^*(t_n) + k(\mathbf{b}^T \otimes I)U^{*'}(t_n)] + k(\mathbf{b}^T \otimes I)(A_h P_h - P_h A)U^*(t_n) + k(\mathbf{b}^T \otimes I)(F_h^* - P_h F^*)(t_n) + \delta_{h,n+1}.$$

As $u^*(t_{n+1}) - u^*(t_n) - k(\mathbf{b}^T \otimes I)U^{*'}(t_n) = O(k^{p+1})$, then

$$(5.11) \quad \delta_{h,n+1} = -k(\mathbf{b}^T \otimes I)(A_h P_h - P_h A)U^*(t_n) - k(\mathbf{b}^T \otimes I)(F_h^* - P_h F^*)(t_n) + O(k^{p+1}).$$

For the numerical solution $\bar{u}_{h,n+1}^*$ of (5.4) starting from $P_h u^*(t_n)$ we have

$$(5.12) \quad \bar{u}_{h,n+1}^* = P_h u^*(t_n) + k(\mathbf{b}^T \otimes A_h)\bar{U}_{h,n}^* + k(\mathbf{b}^T \otimes I)F_h^*(t_n).$$

Subtracting (5.12) from (5.10) we get

$$P_h u^*(t_{n+1}) - \bar{u}_{h,n+1}^* = (\mathbf{b}^T \otimes kA_h) (P_h U^*(t_n) - \bar{U}_{h,n}^*) + \delta_{h,n+1},$$

which, after using (5.9) and (5.11) and some manipulations, leads to

$$(5.13) \quad P_h u^*(t_{n+1}) - \bar{u}_{h,n+1}^* = K_h^n + L_h^n + M_h^n + N_h^n + O(k^{p+1}),$$

where

$$K_h^n = (\mathbf{b}^T \otimes kA_h)(I - k\mathcal{A} \otimes A_h)^{-1} \sum_{l=q+1}^p \frac{k^l}{l!} (\mathbf{w}_l \otimes I) P_h u^{*(l)}(t_n),$$

$$L_h^n = -k\mathbf{b}^T(I - k\mathcal{A} \otimes A_h)^{-1}(F_h^* - P_h F^*)(t_n),$$

$$M_h^n = -k\mathbf{b}^T(I - k\mathcal{A} \otimes A_h)^{-1}[I \otimes (A_h P_h - P_h A)](U^*(t_n) - (\mathbf{e} \otimes I)u^*(t_n)),$$

and

$$N_h^n = -k\mathbf{b}^T(I - k\mathcal{A} \otimes A_h)^{-1}[I \otimes (A_h P_h - P_h A)](\mathbf{e} \otimes I)u^*(t_n) = (I - r(kA_h))A_h^{-1}(A_h P_h - P_h A)(\mathbf{e} \otimes I)u^*(t_n).$$

Now the variation-of-constants formula applied to (5.5) reads

$$(5.14) \quad e_{h,n}^* = r(kA_h)^n [P_h u_0^* - u_{h,0}^*] + \sum_{j=1}^n r(kA_h)^{n-j} [K_h^j + L_h^j + M_h^j + N_h^j] + O(k^p).$$

The first term on the right-hand side of (5.14) can be bounded by $O(\rho\psi_r(h))$.

The term K_h^j turns out to be $O(k^{p+1})$. To see this, notice that the equality

$$A_h^l P_h u^{*(l)} = P_h A^l u^{*(l)} + \sum_{m=1}^l A_h^m A_h^{-1} (A_h P_h - P_h A) A^{l-m} u^{*(l)},$$

together with (5.1) and (5.2), implies the boundedness of $\|A_h^l P_h u^{*(l)}\|$ for $1 \leq l \leq r$. The proof of Theorem 1 in [5] shows that $K_h^j = O(k^{p+1})$. Then, the contribution of these terms to the error is $O(\rho t_n k^p)$.

On the other hand, $\|L_h^j\|$ behaves as $kO(\psi_r(h))$ and, since

$$\|[I \otimes A_h^{-1}(A_h P_h - P_h A)](U^*(t_n) - (\mathbf{e} \otimes I)u^*(t_n))\| = kO(\varphi_r(h))$$

and the operator $\mathbf{b}^T(I - \mathcal{A} \otimes kA_h)^{-1}(kA_h)$ is bounded, the term M_h^j behaves as $k\varphi_r(h)$. Therefore, these terms contribute to the error with

$$\rho t_n (O(\psi_r(h)) + O(\varphi_r(h))).$$

It remains to analyze

$$(5.15) \quad \sum_{j=1}^n r(kA_h)^{n-j} N_h^j$$

which, after summation by parts, can be written as

$$\begin{aligned} & \sum_{j=1}^{n-1} r(kA_h)^{n-j} A_h^{-1}(A_h P_h - P_h A)(\mathbf{e} \otimes I)(u^*(t_j) - u^*(t_{j+1})) \\ & + A_h^{-1}(A_h P_h - P_h A)u^*(t_n) - r(kA_h)^n A_h^{-1}(A_h P_h - P_h A)u^*(t_1). \end{aligned}$$

As long as (5.1) is satisfied and $\|u^*(t_j) - u^*(t_{j+1})\| = O(k)$, then the norm of (5.15) is $\rho t_n O(\varphi_r(h))$. □

Remark 5.2. When using finite elements in the context of the maximum norm, it turns out that the norms in (5.2) behave like $\lambda(h) = O(|\ln h|^{\bar{s}})$, where $\bar{s} = s + 1$, for piecewise linear elements, or $\bar{s} = s$, for higher order elements [33]. This is not a serious problem since $\lambda = \lambda(h)$ enters as a factor in the error constant C in Theorem 5.1.

Remark 5.3. For simplicity we have assumed that the fully discrete scheme is stable. In practice, ρ might depend on h and k . This dependence has been widely studied in the literature (see references in Remark 3.5 and, for second-order elliptic operators and the maximum norm, [7] for finite differences and [27, 34, 36] for finite elements). Typically ρ exhibits at most weak singularities when h and k go to 0. Thus, as ρ enters again as a factor in C , the full order of convergence could be slightly spoiled, due to stability reasons.

Remark 5.4. If $r(\infty) \neq 1$, then the optimal order p may be achieved with $r = p - q - 1$ (see Remark 3.3).

Remark 5.5. Fixed step-sizes are required for the treatment of (5.15), when summation by parts applies. However, in cases for which

$$\|(A_h P_h - P_h A)u^*(t)\| = O(\varphi_r(h))$$

(for instance when finite differences are used), the joint contribution $M_h^n + N_h^n$ can be analyzed without using summation by parts. In these situations variable step-sizes are also allowed.

Remark 5.6. If $\widetilde{W}_1 \subset W_\mu$, $0 < \mu < 1$, and $r < p - q$, then a fractional order in time occurs as in Remark 3.4. In fact, by interpolating the two inequalities

$$\|A_h P_h \xi\| \leq \lambda \|\xi\| + \|P_h\| \|A \xi\|,$$

$$\|P_h \xi\| \leq \|P_h\| \|\xi\|,$$

$\xi \in W_1$, we deduce that when $\|P_h\| = O(1)$ (a standard situation),

$$\|(\omega - A_h)^{\mu'} P_h \xi\| \leq C_{\mu'} \|\xi\|_{\mu},$$

$\xi \in W_{\mu}$, for all $\mu' < \mu$. Thus, an extra order μ' is present for all $\mu' < \mu$. This explains why the extra order μ is observed in full discretizations of (3.2) (see, e.g., the numerical experiments in [24]).

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