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How to avoid order reduction when Lawson methods integrate nonlinear initial boundary value problems

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Abstract It is well known that Lawson methods suffer from a severe order reduction when integrating initial boundary value problems where the solutions are not periodic in space or do not satisfy enough conditions of annihilation on the boundary. However, in a previous paper, a modification of Lawson quadrature rules has been suggested so that no order reduction turns up when integrating linear problems subject to time-dependent boundary conditions. In this paper, we describe and thoroughly analyse a technique to avoid also order reduction when integrating nonlinear problems. This is very useful because, given any Runge-Kutta method of any classical order, a Lawson method can be constructed associated to it for which the order is conserved.

Keywords order reduction · Lawson methods · reaction-diffusion · initial boundary value problems

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1 Introduction

There is an effort in the recent literature to understand the order reduction which turns up when integrating initial boundary value problems subject to non-periodic

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boundary conditions with exponential methods. In that sense, we mention the papers [2,5,11] which correspond to the integration of linear differential problems by Lawson and standard exponential quadrature rules and also through splitting integrators. Understanding this well has led to the design of techniques to avoid that order reduction for both linear and nonlinear problems when the boundary conditions are not only non-periodic but also time-dependent. In that way, for linear problems, suitable modifications of Lawson and exponential quadrature rules have been seen to lead to the order of the underlying classical quadrature rule, as high as desired [3,5]. However, with exponential splitting methods, up to our knowledge, just order 2 has been achieved for the moment for both linear and nonlinear problems [1,4,6,9,10]. As for exponential Runge-Kutta methods [15], stiff order conditions have been deduced to get a given order when integrating semilinear parabolic problems with vanishing boundary conditions [13]. Apart from not considering non-vanishing boundaries there, this implies imposing restrictions on the coefficients of the methods, which may increase the number of stages and therefore the computational cost [17].

As Lawson methods of classical order as high as desired can be constructed directly from any chosen Runge-Kutta method of that order [16], our aim in this paper is to devise a technique to avoid the order reduction which turns up when integrating nonlinear reaction-diffusion initial boundary value problems with Lawson methods and to recover, in such a way, the classical order. The standard approach consists of integrating firstly in space and then in time. With linear problems and vanishing boundary conditions, this has been proved to lead to order 1 in parabolic problems [2]. With non-vanishing boundary conditions, the behaviour is even worse and, even for linear problems, there may be no convergence at all or the error may diminish with the time stepsize but grow with the space grid [3]. There are always exceptions; for example, when considering boundary conditions which are periodic or which satisfy enough conditions of annihilation on the boundary [2] (see also Remarks 3.2, 4.1 and 5.1 in this paper). However, in this paper the main aim is to avoid the strong order reduction which turns up in the general case.

On the other hand, with our proposal, when integrating firstly in time, some terms of Lawson method are calculated through the solution of linear initial boundary value problems for which suitable boundary values are chosen. Then, the space discretization of those problems must be performed. The main achievement of the paper is how to choose those boundary values in order to get a given accuracy and how to calculate them in terms of the given data of the problem. More precisely, with any consistent RK method, we prove that local order 2 can be achieved by calculating the boundary values exactly in terms of the given data for Dirichlet boundary conditions or in an approximate way (through the numerical solution) for Neumann/Robin ones. In any case, to obtain local order 2, there is no need to resort to numerical differentiation. Besides, if the RK method has order ≥ 2, global order 2 is achieved if the summation-by-parts argument is applied. Look at [12] (page 226) for a stiff ordinary differential equation where already local and global order coincide with a similar argument, and at [2] to see the same phenomenon when integrating linear parabolic initial boundary value problems with Lawson methods. Moreover, by resorting to numerical differentiation, local order 3 can be achieved with these methods whose underlying Runge-Kutta has classical second order and, whenever a CFL condition is

satisfied (4.4), global order ≥ 2 and smaller errors are obtained. (We remark that this condition is not very restrictive in the sense that, when the differential problem is of second-order in space and the boundary conditions are Dirichlet, $\gamma = 1$ in (4.4) and therefore it just means that the time stepsize is not too big with respect to the space grid. With Robin/Neumann boundary conditions and the same type of differential operator, $\gamma = 0$ and no CFL restriction would even turn up.) Up to our knowledge, it is the first time in the literature in which the error coming from numerical differentiation is thoroughly considered in the analysis. Finally, although the formulas get more complicated, by using numerical differentiation, local order 4 can also be achieved if the underlying RK method is of order ≥ 3. We have not described the formulas to get local order ≥ 5 because they get more and more complicated, because there are less problems where so much accuracy is required, and also due to the fact that numerical differentiation is ill-posed [19], and therefore the rounding errors associated to their use might cause that not so much accuracy is achieved.

The paper is structured as follows. Section 2 gives some preliminaries on the abstract framework for the problem, on Lawson methods and on the assumptions we make for the space discretization. The technique to avoid order reduction is suggested in Sections 3, 4 and 5, separating the cases in which we want to achieve local orders 2, 3 and 4. The final formulas to be implemented are respectively (3.6), (4.2) and (5.1) and, in Remark 3.1 and Subsections 4.1 and 5.1, a thorough discussion is given on how to calculate the required suggested boundaries for either Dirichlet, Robin or Neumann boundary conditions. Finally, some numerical results are shown in Section 6 which corroborate the theoretical results and prove the great improvement of the method suggested against the standard approach. For the sake of brevity and readability, we just show here the precise proofs of some of the theorems, which have been postponed to an appendix.

2 Preliminaries

Let X and Y be Banach spaces and let $A : D(A) \subset X \to X$ and $\partial : D(A) \to Y$ be linear operators. Our goal is to avoid order reduction when integrating in time through Lawson methods the nonlinear abstract non-homogeneous initial boundary value problem

$$\begin{aligned} u'(t) &= Au(t) + f(t,u(t)), \quad 0 \leq t \leq T, \\ u(0) &= u_0 \in X, \\ \partial u(t) &= g(t) \in Y, \quad 0 \leq t \leq T. \end{aligned} \tag{2.1}$$

We will assume that the functions $f : [0,T] \times X \to X$ (in general nonlinear) and $g : [0,T] \to Y$ are regular enough.

The abstract setting (2.1) permits to cover a wide range of nonlinear evolutionary problems governed by partial differential equations. We use the following hypotheses, similar to the ones made in [4] to avoid order reduction when integrating the same kind of problems with exponential splitting methods.

(A1) $\partial : D(A) \subset X \to Y$ is onto and $g \in C^1([0,T],Y)$.

(A2) Ker(∂) is dense in X and $A_0 = A|_{Ker(\partial)}$ is the infinitesimal generator of a C_0-semigroup $\{e^{tA_0}\}_{t\geq 0}$ in X of negative type ω.

(A3) If $z \in \mathbf{C}$ satisfies $\Re(z) > \omega$ and $v \in Y$, then the problem

$$Ax = zx, \tag{2.2}$$

$$\partial x = v, \tag{2.3}$$

has a unique solution ($x = K(z)v$) which satisfies

$$\|K(z)v\| \leq C\|v\|, \tag{2.4}$$

where the constant C holds for any z such that $Re(z) \geq \omega_0 > \omega$.

(A4) $f \in C^1([0,T]\times X, X)$.

(A5) $u \in C^1([0,T],X)$, $u(t) \in D(A)$ for all $t \in [0,T]$ and $Au \in C([0,T],X)$.

The well-posedness of problem (2.1) is assured by (A1)-(A4), as explained in [4]. Besides, as it was also justified there, (A4) is quite restrictive in an L^p Banach space. However, if the supremum norm is chosen, (A4) is satisfied whenever f has the form

$$f(t,u) = \phi(u) + h(t), \tag{2.5}$$

with $\phi \in C^1(\mathbf{C},\mathbf{C})$ and $h \in C^1([0,T],X)$. For simplicity, we will assume from now on that f has the form (2.5), and also that the following hypotheses are satisfied:

(A6) ϕ is such that, whenever $w \in D(A^l)$ for natural number l, $\phi(w)$ and $\phi'(w)$ also belong to $D(A^l)$.

(A7) For natural l and j, whenever $r \in C^j([0,T],X)$ with $r(t) \in D(A^l)$ for every $t \in [0,T]$, it follows that $A^l r, A^l\phi(r) \in C^j([0,T],X)$.

Notice that, when A is a space differential operator, (A6) means that ϕ and ϕ' do not reduce the regularity in space of their arguments. As for (A7), it means that the regularity in time is not disturbed by that in space. In the remaining of the paper, we always suppose that (A1)-(A7) are satisfied. However, more regularity will be assumed in certain results.

Because of hypothesis (A2), $\{\varphi_j(tA_0)\}_{j=1}^3$ are bounded operators for $t > 0$, where $\{\varphi_j\}$ are the standard functions which are used in exponential methods [15] and which are defined by

$$\varphi_j(tA_0) = \frac{1}{t^j}\int_0^t e^{(t-\tau)A_0}\frac{\tau^{j-1}}{(j-1)!}d\tau, \quad j \geq 1. \tag{2.6}$$

They can also be recursively defined through the formulas

$$\varphi_{j+1}(z) = \frac{\varphi_j(z) - 1/j!}{z}, \quad z \neq 0, \qquad \varphi_{j+1}(0) = \frac{1}{(j+1)!}, \qquad \varphi_0(z) = e^z. \tag{2.7}$$

For the time integration, we will center on exponential Lawson methods which are determined by an explicit Runge-Kutta tableau and which, when applied to a finite-dimensional nonlinear problem like

$$U'(t) = MU(t) + F(t,U(t)), \tag{2.8}$$

where M is a matrix, read like this at each step

$$K_{n,i} = e^{c_i kM} U_n + k \sum_{j=1}^{i-1} a_{ij} e^{(c_i - c_j)kM} F(t_n + c_j k, K_{n,j}), \quad i = 1, \ldots, s, \tag{2.9}$$

$$U_{n+1} = e^{kM} U_n + k \sum_{i=1}^{s} b_i e^{(1-c_i)kM} F(t_n + c_i k, K_{n,i}), \tag{2.10}$$

where $k > 0$ is the time stepsize and $t_n = t_0 + nk$. We will assume that the coefficients of Butcher tableau satisfy the following standard equalities:

$$\sum_{i=1}^{s} b_i = 1 \text{ (consistency)}, \qquad \sum_{j=1}^{i-1} a_{ij} = c_i, \ i = 1, \ldots, s. \tag{2.11}$$

Following the example in Section 2 of [4], we take $X = C(\overline{\Omega})$ for a certain bounded domain $\Omega \in \mathbf{R}^d$. There, we consider the maximum norm and a certain grid Ω_h (of Ω) over which the approximated numerical solution will be defined. In this way, this numerical approximation belongs to C^N, where N is the number of nodes in the grid, and the maximum norm $\|u_h\|_h = \|[u_1, \ldots, u_N]^T\|_h = \max_{1 \le i \le N} |u_i|$ is considered.

Notice that, when dealing with Dirichlet boundary conditions, the values at nodes on the boundary are not subject to numerical approximation since we already know the exact values there while, with Neumann or Robin boundary conditions, an approximation for the values at those nodes is usually given.

We denote by

$$P_h : X \to \mathbf{C}^N, \tag{2.12}$$

the nodal projection on the grid Ω_h. As for the discretization of the operator A, we consider

$$A_{h,0} U_h + C_h g,$$

where $A_{h,0}$ is the matrix which discretizes A_0 and $C_h : Y \to \mathbf{C}^N$ is the operator which takes the boundary information $\partial u = g$.

Notice that, as the source function f is given by (2.5), it can also be understood as a function from $[0,T] \times \mathbf{C}^N$ on $\mathbf{C}^N$ and, for each $t \in [0,T]$ and $u \in X$,

$$P_h f(t,u) = f(t, P_h u). \tag{2.13}$$

In a similar way to [4], in the rest of the paper we consider the following hypotheses:

(H1) $A_{h,0}$ is such that
  (a) $\|e^{tA_{h,0}}\|_h \le 1$,
  (b) $A_{h,0}$ is invertible and $\|A_{h,0}^{-1}\|_h$ is uniformly bounded on h.
  This hypothesis is related to (A2) for the continuous problem.

(H2) We define the elliptic projection $R_h : D(A) \to \mathbf{C}^N$ as the solution of

$$A_{h,0}R_h u + C_h \partial u = P_h A u. \tag{2.14}$$

We assume that, for a certain subspace $Z \subset D(A)$, it follows that:

(a) For $u \in Z$, $A_0^{-1}u \in Z$ and $e^{tA_0}u, f(t,u) \in Z$, for $t \in [0,T]$.
Whenever $w \in D(A^l)$ with $A^l w \in Z$, $A^l \phi(w) \in Z$.
Whenever $r \in C^1([0,T], D(A^l))$, with $A^l r(t) \in Z$ for every $t \in [0,T]$,
$A^l \dot{r}(t), A^l \phi(r(t)), A^l \phi'(r(t))w \in Z$ for every $t \in [0,T]$ and $w \in Z$.

(b) For some ε_h and η_h decreasing with h,

$$\left\| A_{h,0}(P_h u - R_h u) \right\| \leq \varepsilon_h \|u\|_Z, \quad \|P_h u - R_h u\| \leq \eta_h \|u\|_Z. \tag{2.15}$$

These assumptions are related to the fact that, in order to get a given accuracy after the space discretization of an elliptic problem, some extra regularity is required. Look at Section 6 for an example.

(c) $\|A_{h,0}^{-1} C_h\|_h \leq C''$ is uniformly bounded on h. This corresponds to the discrete maximum principle associated to the continuous one (2.4) when $z = 0$.

As in [4], hypothesis (H1a) can be deduced in our numerical experiments by using the logarithmic norm of matrix $A_{h,0}$.

Notice that, by using the space discretization which is described previously, the following semidiscrete problem arises after discretising (2.1),

$$\begin{aligned} U_h'(t) &= A_{h,0}U_h(t) + C_h g(t) + f(t, U_h(t)), \\ U_h(t_0) &= P_h u(t_0). \end{aligned} \tag{2.16}$$

Then, applying Lawson method (2.9)-(2.10) to this, the following formulas define one step from U_h^n to U_h^{n+1}:

$$\begin{aligned} K_{h,i}^n &= e^{c_i k A_{h,0}} U_h^n + k \sum_{j=1}^{i-1} a_{ij} e^{(c_i - c_j) k A_{h,0}} [C_h g(t_n + c_j k) + f(t_n + c_j k, K_{h,j}^n)], \\ U_h^{n+1} &= e^{k A_{h,0}} U_h^n + k \sum_{i=1}^{s} b_i e^{(1-c_i) k A_{h,0}} [C_h g(t_n + c_i k) + f(t_n + c_i k, K_{h,i}^n)]. \end{aligned} \tag{2.17}$$

This corresponds to the standard method of lines which was already proved to lead to strong order reduction in [2] for linear problems and vanishing boundary conditions. In a more precise way, for the nonlinear problems under consideration in this paper, in [7] it is proved that just order 1 in time (uniformly in space) turns up with general vanishing boundary conditions. As for non-vanishing ones, either order 1 in time occurs (but not uniformly in space, so that the errors rapidly grow when the space grid diminishes) or even no convergence in time is observed.

3 Searching for local order 2

Our approach consists of discretizing firstly in time and then in space. When discretizing in time, some attention must be given to the exponential terms which turn up in Lawson formulas (2.9)-(2.10). If $u(t_n)$ or f evaluated at the stages vanished at the boundary, it could seem natural to substitute those exponential operators by the C_0-semigroup $e^{\tau A_0}$ for suitable scalar values τ. However, that may also lead to order reduction since the solution of

$$\dot{u}(\tau) = A_0 u(\tau), \quad u(0) = \alpha,$$

cannot be accurately enough approximated by an expansion of the form

$$u_0 + \tau A_0 \alpha + \frac{\tau^2}{2} A_0^2 \alpha + \cdots$$

unless $\alpha \in D(A_0^l)$ for a high enough l. Besides, as $u(t_n)$ or f evaluated at the stages do not vanish in general, the solution of suitable initial boundary value problems must be considered as candidates for each exponential term. More precisely, boundary values must be chosen which approximate till a given order the exponential function in some way.

We will consider three different cases depending on whether we want to achieve local order 2, 3 or 4. For local order 2 and Dirichlet boundary conditions, those boundaries can be calculated directly in terms of the data f and g of the problem (2.1). For the same order, but with Neumann/Robin boundary conditions, the approximation at the boundary given by the space discretization of the problem must be used. For higher orders, we will have to resort to numerical differentiation to calculate those boundaries.

The main difference with respect to the linear case is that now the stages have a role. More precisely, in order to get local order 2, starting from the continuous approximation u_n at $t = t_n$, we consider recursively for the stages:

$$K_{n,i} = v_n(c_i k) + k \sum_{j=1}^{i-1} a_{ij} w_{n,j}((c_i - c_j)k), \quad i = 1, \ldots, s, \tag{3.1}$$

where

$$\begin{cases} \dot{v}_n(\sigma) = A v_n(\sigma), \\ v_n(0) = u_n, \\ \partial v_n(\sigma) = \partial u(t_n), \end{cases} \quad \begin{cases} \dot{w}_{n,j}(\sigma) = A w_{n,j}(\sigma), \\ w_{n,j}(0) = f(t_n + c_j k, K_{n,j}), \\ \partial w_{n,j}(\sigma) = 0, \end{cases} \tag{3.2}$$

Notice that we are more accurate in handling the boundary conditions for v_n than for $w_{n,j}$ because of the factor k before the sum in (3.1). Then, we suggest as the numerical approximation at the next step

$$u_{n+1} = \tilde{v}_n(k) + k \sum_{i=1}^{s} b_i \tilde{w}_{n,i}((1 - c_i)k), \tag{3.3}$$

where

$$\left\{\begin{array}{l}\dot{\tilde{v}}_n(\sigma)=A\tilde{v}_n(\sigma),\\ \tilde{v}_n(0)=u_n,\\ \partial\tilde{v}_n(\sigma)=\partial[u(t_n)+\sigma Au(t_n)],\end{array}\right. \qquad \left\{\begin{array}{l}\dot{\tilde{w}}_{n,j}(\sigma)=A\tilde{w}_{n,j}(\sigma),\\ \tilde{w}_{n,j}(0)=f(t_n+c_jk,K_{n,j}),\\ \partial\tilde{w}_{n,j}(\sigma)=\partial f(t_n,u(t_n)).\end{array}\right. \tag{3.4}$$

Notice that we are again more accurate in the boundary for $\tilde{v}_n$ than for $\tilde{w}_{n,j}$ and, in any case, we are one order more accurate than in (3.2) because we are approximating the solution and not just the stages. After discretizing (3.2) and (3.4) in space, the following systems arise when starting from the discrete numerical approximation $U_{n,h}$ at the previous step, and denoting by $K_{n,h,j}$ to the discretized stages,

$$\left\{\begin{array}{l}\dot{V}_{n,h}(\sigma)=A_{h,0}V_{n,h}(\sigma)+C_h\partial u(t_n),\\ V_{n,h}(0)=U_{n,h},\end{array}\right. \quad \left\{\begin{array}{l}\dot{W}_{n,h,j}(\sigma)=A_{h,0}W_{n,h,j}(\sigma),\\ W_{n,h,j}(0)=f(t_n+c_jk,K_{n,h,j}).\end{array}\right.$$

$$\left\{\begin{array}{l}\dot{\tilde{V}}_{n,h}(\sigma)=A_{h,0}\tilde{V}_{n,h}(\sigma)+C_h[\partial u(t_n)+\sigma Au(t_n)],\\ \tilde{V}_{n,h}(0)=U_{n,h},\end{array}\right.$$

$$\left\{\begin{array}{l}\dot{\tilde{W}}_{n,h,j}(\sigma)=A_{h,0}\tilde{W}_{n,h,j}(\sigma)+C_h\partial f(t_n,u(t_n)),\\ \tilde{W}_{n,h,j}(0)=f(t_n+c_jk,K_{n,h,j}).\end{array}\right. \tag{3.5}$$

By using the variation-of-constants formula and the definition of φ_j in (2.6), we have

$$\begin{aligned}V_{n,h}(\sigma)&=e^{\sigma A_{h,0}}U_{n,h}+\int_0^\sigma e^{(\sigma-\tau)A_{h,0}}C_h\partial u(t_n)d\tau=e^{\sigma A_{h,0}}U_{n,h}+\sigma\varphi_1(\sigma A_{h,0})C_h\partial u(t_n),\\ \tilde{V}_{n,h}(\sigma)&=e^{\sigma A_{h,0}}U_{n,h}+\sigma\varphi_1(\sigma A_{h,0})C_h\partial u(t_n)+\sigma^2\varphi_2(\sigma A_{h,0})C_h\partial Au(t_n),\\ \tilde{W}_{n,h,j}(\sigma)&=e^{\sigma A_{h,0}}f(t_n+c_jk,K_{n,h,j})+\sigma\varphi_1(\sigma A_{h,0})C_h\partial f(t_n,u(t_n)).\end{aligned}$$

Therefore, considering (3.1) and (3.3), the full discretized numerical solution after one step is calculated recursively through the following formulas

$$\begin{aligned}K_{n,h,i}&=e^{c_ikA_{h,0}}U_{n,h}+c_ik\varphi_1(c_ikA_{h,0})C_h\partial u(t_n)+k\sum_{j=1}^{i-1}a_{ij}e^{(c_i-c_j)kA_{h,0}}f(t_n+c_jk,K_{n,h,j}),\\ U_{n+1,h}&=e^{kA_{h,0}}U_{n,h}+k\varphi_1(kA_{h,0})C_h\partial u(t_n)+k^2\varphi_2(kA_{h,0})C_h\partial Au(t_n)\\ &\quad+k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}f(t_n+c_ik,K_{n,h,i})\\ &\qquad+(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_h\partial f(t_n,u(t_n))\Big].\end{aligned} \tag{3.6}$$

Remark 3.1 Notice that the three terms on the boundary $\partial u(t_n)$, $\partial Au(t_n)$ and $\partial f(t_n,u(t_n))$, are necessary to consider this approximation. However, as

$$\partial u(t_n)=g(t_n),\quad \partial Au(t_n)=\dot{g}(t_n)-\partial f(t_n,u(t_n)),$$

all reduces to calculate $\partial f(t_n,u(t_n))$. In the same way as it was stated in [4,10], with Dirichlet boundary conditions, using (2.5), that term can be calculated exactly as

$$\partial f(t_n,u(t_n))=\phi(g(t_n))+\partial h(t_n).$$

With Neumann or Robin boundary conditions

$$\partial u(t) = \alpha u(t)|_{\partial\Omega} + \beta \partial_n u(t)|_{\partial\Omega} = g(t), \quad \beta \neq 0, \tag{3.7}$$

as

$$\partial f(t_n, u(t_n)) = \alpha[\phi(u(t_n)|_{\partial\Omega}) + h(t_n)|_{\partial\Omega}] + \beta[\phi'(u(t_n)|_{\partial\Omega})\partial_n u(t_n)|_{\partial\Omega} + \partial_n h(t_n)|_{\partial\Omega}],$$

$u(t_n)|_{\partial\Omega}$ can be approximated by the numerical solution which the space discretization of the problem necessarily gives in this case and $\partial_n u(t_n)|_{\partial\Omega}$ by the result of solving from (3.7). Notice that, with this type of boundary condition, the grid where the solution is approximated contains nodes on the boundary. Those approximated nodal values are usually the ones which C_h needs to calculate $C_h \partial f(t_n, u(t_n))$. In any case, the error which comes from the approximation of the boundary terms in (3.6) is given in Table 4.1.

Remark 3.2 We also notice that, when $\partial u(t) = \partial A u(t) = 0$, because of (2.1), it necessarily happens that $\partial f(t, u(t)) = 0$. Besides, in this case, (3.6) is equivalent to (2.17). In this way, through Theorems 3.1 and 3.2, we will be implicitly proving local order 2 for the standard approach in such a case.

3.1 Local error of the time semidiscretization

In order to define the local error of the time semidiscretization, we consider

$$\begin{aligned} \bar{K}_{n,i} &= \bar{v}_n(c_i k) + k \sum_{j=1}^{i-1} a_{ij} \bar{w}_{n,j}((c_i - c_j)k), \quad i = 1, \ldots, s, \\ \bar{u}_{n+1} &= \bar{\bar{v}}_n(k) + k \sum_{i=1}^{s} b_i \bar{\bar{w}}_{n,i}((1 - c_i)k), \end{aligned} \tag{3.8}$$

where $\bar{v}_n$ and $\bar{\bar{v}}_n$ satisfy the same equation and boundary conditions as v_n and $\tilde{v}_n$, but starting from $u(t_n)$ instead of u_n. The same happens with $\bar{w}_{n,i}$, $\bar{\bar{w}}_{n,i}$ and $w_{n,i}$, $\tilde{w}_{n,i}$ with the difference that the initial condition is now $f(t_n + c_i k, \bar{K}_{n,i})$ instead of $f(t_n + c_i k, K_{n,i})$. Then, for the local error $\rho_n = \bar{u}_{n+1} - u(t_{n+1})$, the following theorem can be stated, as it is proved in the appendix.

Theorem 3.1 *Assuming that*

$$h \in C^1([0,T], D(A)), \quad u \in C^2([0,T], D(A^2)), \tag{3.9}$$

it follows that $\rho_n = O(k^2)$. Moreover, if $f \in C^2([0,T] \times X, X), u \in C^3([0,T], X)$, there exists a constant C such that the following bound holds

$$\|A_0^{-1} f_u(t, u(t)) A_0 w\| \leq C\|w\|, \text{ for every } t \in [0,T],\ w \in D(A_0), \tag{3.10}$$

and the Runge-Kutta tableau corresponds to a method of classical order ≥ 2, it follows that $A_0^{-1}\rho_n = O(k^3)$.

3.2 Local error of the full discretization

We define the local error of the full discretization as $\rho_{n+1,h} = \bar{U}_{n+1,h} - P_h u(t_{n+1})$, where $\bar{U}_{n+1,h}$ is defined as $U_{n+1,h}$ but starting from $P_h u(t_n)$. The next result then follows, with similar arguments as those in [4] for splitting methods, as it is thoroughly shown in [7]:

Theorem 3.2 *Under the same hypotheses of the first part of Theorem 3.1, and assuming also that, for $t \in [0,T]$,*

$$A^l u(t) \in Z, \quad l = 0,1,2, \qquad A^l h(t) \in Z, \quad l = 0,1, \quad t \in [0,T], \tag{3.11}$$

it holds that $\rho_{n,h} = O(k^2 + k\varepsilon_h)$ where ε_h is that in (2.15). Moreover, under the additional hypotheses of the second part of Theorem 3.1, together with the following condition which is related to (3.10),

$$\|A_{h,0}^{-1} f_u(t, P_h u(t)) A_{h,0}\|_h \leq C, \quad t \in [0,T], \quad h \leq h_0, \tag{3.12}$$

it follows that $A_{h,0}^{-1}\rho_{n,h} = O(k^3 + k\eta_h + k^2\varepsilon_h)$, where η_h is that in (2.15).

3.3 Global error of the full discretization

From the first part of Theorem 3.2, the classical argument would lead to global error $e_{n,h} = U_{n,h} - P_h u(t_n) = O(k + \varepsilon_h)$. However, for parabolic problems, for which this bound is expected to hold (see [14]),

$$\|kA_{h,0} \sum_{r=1}^{n-1} e^{rkA_{h,0}}\|_h \leq C, \quad 0 \leq nk \leq T, \tag{3.13}$$

using the second part of the same theorem, a summation-by-parts argument leads to second order in time, as the following theorem states. The theorem is valid for both Dirichlet and Neumann/Robin boundary conditions, in spite of the fact that, for the latter, $\partial f(t,u(t))$ must be approximated through the numerical solution itself, as explained in Remark 3.1. The proof of the theorem is again in the appendix.

Theorem 3.3 *Under hypotheses of Theorem 3.2, but assuming also (3.13) and that*

$$\begin{aligned} &\phi \in C^3(\mathbf{C},\mathbf{C}),\ h \in C^3([0,T],D(A)),\ u \in C^4([0,T],D(A^2)),\\ &A^l \dot{u}(t) \in Z,\ l = 0,1,2, \quad A^l h(t) \in Z,\ l = 0,1, \quad t \in [0,T], \end{aligned}$$

it follows that $e_{n,h} = U_{n,h} - P_h u(t_n) = O(k^2 + k\varepsilon_h + \eta_h)$.

4 Searching for local order 3

For the stages, we again consider (3.1), but where now we are one order more accurate for the boundaries of v_n and $w_{n,j}$. In this manner, the latter can be calculated through (3.4) instead of (3.2). On the other hand, u_{n+1} is calculated through (3.3) where now $\tilde{v}_n$, $\tilde{w}_{n,j}(j=1,\ldots,s)$ satisfy

$$\begin{cases} \dot{\tilde{v}}_n(\sigma) = A\tilde{v}_n(\sigma), \\ \tilde{v}_n(0) = u_n, \\ \partial\tilde{v}_n(\sigma) = \partial[u(t_n)+\sigma Au(t_n)+\frac{\sigma^2}{2}A^2u(t_n)], \end{cases}$$
$$\begin{cases} \dot{\tilde{w}}_{n,j}(\sigma) = A\tilde{w}_{n,j}(\sigma), \\ \tilde{w}_{n,j}(0) = f(t_n+c_jk,K_{n,j}), \\ \partial\tilde{w}_{n,j}(\sigma) = \partial[f(t_n+c_jk,u(t_n)+c_jk\dot{u}(t_n))+\sigma Af(t_n,u(t_n))]. \end{cases} \tag{4.1}$$

After discretizing in space and using the variation-of-constants formula, as we did in Section 3, the full discretized numerical solution after one step is given by

$$\begin{aligned} K_{n,h,i} &= e^{c_ikA_{h,0}}U_{n,h}+c_ik\varphi_1(c_ikA_{h,0})C_h\partial u(t_n)+c_i^2k^2\varphi_2(c_ikA_{h,0})C_h\partial Au(t_n) \\ &\quad +k\sum_{j=1}^{i-1}a_{ij}\Big[e^{(c_i-c_j)kA_{h,0}}f(t_n+c_jk,K_{n,h,j}) \\ &\qquad +(c_i-c_j)k\varphi_1((c_i-c_j)kA_{h,0})C_h\partial f(t_n,u(t_n))\Big], \quad i=1,\ldots,s, \\ U_{n+1,h} &= e^{kA_{h,0}}U_{n,h}+\sum_{l=1}^{3}k^l\varphi_l(kA_{h,0})C_h\partial A^{l-1}u(t_n) \\ &\quad +k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}f(t_n+c_ik,K_{n,h,i}) \\ &\qquad +(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_h\partial f(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n)) \\ &\qquad +(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_h\partial Af(t_n,u(t_n))\Big]. \end{aligned} \tag{4.2}$$

Remark 4.1 We notice that, if $\partial u(t)=\partial Au(t)=\partial A^2u(t)=0$, from (2.1) it follows that $\partial f(t,u(t))=\partial Af(t,u(t))=0$. In particular, this implies that $\partial f(t_n+c_ik,u(t_n+c_ik))=0$, which differs from $\partial f(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n))$ in $O(k^2)$. Then, in this case, each step in (4.2) differs from the standard approach (2.17) in $O(k^3)$ since the difference is

$$k\sum_{i=1}^{s}b_i(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_hO(k^2)=k\sum_{i=1}^{s}b_i[e^{(1-c_i)kA_{h,0}}-I]A_{h,0}^{-1}C_hO(k^2),$$

and, according to (H2c), $A_{h,0}^{-1}C_h$ is uniformly bounded. This justifies, through Theorems 4.1 and 4.2, that the local error with the standard approach, under these particular boundary conditions, behaves with order 3 under the assumptions of those theorems.

4.1 Calculation or approximation of the boundaries which are required to achieve local order 3

Notice that, apart from the terms on the boundary which were already necessary to achieve local order 2 and which can be calculated according to Remark 3.1, now we also need $\partial A^2 u(t_n)$, $\partial f(t_n + c_i k, u(t_n) + c_i k \dot{u}(t_n))$ and $\partial A f(t_n, u(t_n))$.

With Dirichlet boundary conditions, using (2.5), it follows that

$$\begin{aligned} \partial f(t_n + c_i k, u(t_n) + c_i k \dot{u}(t_n)) &= \phi(g(t_n) + c_i k \dot{g}(t_n)) + \partial h(t_n + c_i k), \\ \partial A^2 u(t_n) &= \ddot{g}(t_n) - \partial \dot{h}(t_n) - \phi'(g(t_n)) \dot{g}(t_n) - \partial A f(t_n, u(t_n)), \end{aligned}$$

and the only term that cannot be calculated exactly in terms of data is $\partial A f(t_n, u(t_n))$. However, that can be approximated resorting to numerical differentiation. For example, in one dimension and assuming that A is the second spatial derivative,

$$A f(t_n, u(t_n)) = \phi''(u(t_n)) u_x(t_n)^2 + \phi'(u(t_n)) u_{xx}(t_n) + h_{xx}(t_n),$$

from what

$$\partial A f(t_n, u(t_n)) \approx \phi''(g(t_n)) \hat{u}_x(t_n)^2|_{\partial\Omega} + \phi'(g(t_n))(\dot{g}(t_n) - \phi(g(t_n)) - \partial h(t_n)) + \partial h_{xx}(t_n),$$

where $\hat{u}_x(t_n)|_{\partial\Omega}$ is the result of applying numerical differentiation to approximate $u_x(t_n)$ on the boundary. For that, both the exact values at the boundary and the approximated values at the interior of the domain given by the numerical approximation must be used. As a result, $\hat{u}_x(t_n) - u_x(t_n) = O(\nu_h + \frac{e_{n,h}}{h})$, where ν_h decreases with h and comes from the error of the numerical differentiation if the exact values of the solutions were used. The second term $\frac{e_{n,h}}{h}$ comes from the fact that the values at the interior are just the approximations which are given by the numerical solution and to the necessity of dividing by h when approximating a first derivative in space. For a general operator A, we will assume that the error when approximating both $\partial A^2 u(t_n)$ and $\partial A f(t_n, u(t_n))$ is as specified in Table 4.1 for some real value γ, where ν_h comes from the numerical approximation of the corresponding derivatives in space if the exact values had been taken.

As for Robin/Neumann boundary conditions (3.7), we notice that

$$\begin{aligned} \partial f(t_n + c_i k, u(t_n) + c_i k \dot{u}(t_n)) &= \alpha[\phi(u(t_n)|_{\partial\Omega} + c_i k \dot{u}(t_n)|_{\partial\Omega}) + h(t_n + c_i k)|_{\partial\Omega}] \\ &+ \beta[\phi'(u(t_n)|_{\partial\Omega} + c_i k \dot{u}(t_n)|_{\partial\Omega})(\partial_n u(t_n)|_{\partial\Omega} + c_i k \partial_n \dot{u}(t_n)|_{\partial\Omega}) + \partial_n h(t_n + c_i k)|_{\partial\Omega}]. \end{aligned}$$

Here $u(t_n)|_{\partial\Omega}$ and $\partial_n u(t_n)|_{\partial\Omega}$ are approximated through the numerical solution, as in Remark 3.1, $\dot{u}(t_n)|_{\partial\Omega}$ is approximated through numerical differentiation in time from the approximated values at the boundary and $\partial_n \dot{u}(t_n)|_{\partial\Omega}$ is then solved from the differentiation in time of (3.7). In such a way, if the error coming from the numerical differentiation in time from the exact values is $O(\mu_{k,1})$, with $\mu_{k,1}$ decreasing when k decreases, it happens that the error when approximating $\partial f(t_n + c_i k, u(t_n) + c_i k \dot{u}(t_n))$ is $O(k\mu_{k,1} + e_{n,h})$, with the same argument as before for space numerical differentiation, and taking now into account the factor k which is multiplying the corresponding

Table 4.1 Errors which are committed at each step when approximating the corresponding boundary terms with the suggested technique to avoid order reduction, as justified in Remark 3.1 and Subsections 4.1 and 5.1.

	Dirichlet	Robin/Neumann
$\partial u(t_n)$	-	-
$\partial Au(t_n)/\partial f(t_n,u(t_n))$	-	$O(e_{n,h})$
$\partial f(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n))$	-	$O(k\mu_{k,1}+e_{n,h})$
$\partial A^2u(t_n)/\partial Af(t_n,u(t_n))$	$O(\nu_h+\frac{e_{n,h}}{h^\gamma})$	$O(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})$
$\partial Af(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n))$	$O(\nu_h+\frac{e_{n,h}}{h^\gamma}+\frac{k\mu_{k,1}}{h^\gamma})$	$O(k\mu_{k,1}+k\mu_{k,2}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})$
$\partial A^3u(t_n)/\partial A^2f(t_n,u(t_n))$	$O(\nu_h+\frac{e_{n,h}}{kh^\gamma}+\frac{\mu_{k,1}}{h^\gamma})$	$O(\mu_{k,1}+\mu_{k,2}+\frac{e_{n,h}}{k^2}+\nu_h+\frac{e_{n,h}}{kh^\gamma})$

derivative. As for $\partial A^2u(t_n)$, using (2.1), $\partial A^2u=\ddot{g}-\partial[\dot{h}+\phi'(u)\dot{u}]-\partial(Af)$. Moreover,

$$\begin{aligned}\partial[\dot{h}+\phi'(u)\dot{u}] = {}& \alpha[\dot{h}|_{\partial\Omega}+\phi'(u|_{\partial\Omega})\dot{u}|_{\partial\Omega}]+\beta[\partial_n\dot{h}|_{\partial\Omega}+\phi''(u|_{\partial\Omega})\partial_nu|_{\partial\Omega}\dot{u}|_{\partial\Omega}\\ &+\phi'(u|_{\partial\Omega})\partial_n\dot{u}|_{\partial\Omega}],\end{aligned}$$

and it is then necessary to approximate $u|_{\partial\Omega}$, $\partial_nu|_{\partial\Omega}$, $\dot{u}|_{\partial\Omega}$ and $\partial_n\dot{u}|_{\partial\Omega}$, as before. On the other hand, when A is the second derivative in one dimension,

$$\begin{aligned}\partial(Af) = {}& \alpha\Big[\phi''(u|_{\partial\Omega})u_x^2|_{\partial\Omega}+\phi'(u|_{\partial\Omega})[\dot{u}|_{\partial\Omega}-\phi(u|_{\partial\Omega})-h|_{\partial\Omega}]+h_{xx}|_{\partial\Omega}\Big]\\ &+\beta\Big[\phi'''(u|_{\partial\Omega})u_x^3|_{\partial\Omega}+3\phi''(u|_{\partial\Omega})u_x|_{\partial\Omega}[\dot{u}|_{\partial\Omega}-\phi(u|_{\partial\Omega})-h|_{\partial\Omega}]\\ &\quad+\phi'(u|_{\partial\Omega})[\dot{u}_x|_{\partial\Omega}-\phi'(u|_{\partial\Omega})u_x|_{\partial\Omega}-h_x|_{\partial\Omega}]+h_{xxx}|_{\partial\Omega}\Big].\end{aligned}$$

Therefore, in this particular case, approximating $u|_{\partial\Omega}$, $\dot{u}|_{\partial\Omega}$, $u_x|_{\partial\Omega}$ and $\dot{u}_x|_{\partial\Omega}$ as above, the error which comes from calculating $\partial A^2u(t_n)$ and $\partial Af(t_n,u(t_n))$ is $O(\mu_{k,1}+\frac{e_{n,h}}{k})$. However, for more general operators, space numerical differentiation may be also needed, and therefore we will assume that, in general, the error coming from the calculation of those boundaries is as specified in Table 4.1.

4.2 Local error of the time semidiscretization

When discretizing in time as specified at the beginning of Subsection 4, we have the following result, which is stronger than Theorem 3.1 because more accuracy is being considered with respect to the boundaries of the problems in (3.2) and (3.4). (Its proof is similar to that of Theorem 3.1 and is shown in [7].)

Theorem 4.1 *Assuming that*

$$\phi\in C^2(\mathbf{C},\mathbf{C}),\ h\in C^2([0,T],D(A^2)),\ u\in C^3([0,T],D(A^3)),\tag{4.3}$$

and that the Runge-Kutta tableau corresponds to a method of classical order ≥ 2*, it follows that* $\rho_n = O(k^3)$*. Moreover, if* $f \in C^3([0,T]\times X, X), u \in C^4([0,T], X)$*, (3.10) holds and the Runge-Kutta tableau corresponds to a method of classical order* ≥ 3*, it follows that* $A_0^{-1}\rho_n = O(k^4)$*.*

4.3 Local error of the full discretization

Following a similar proof to that of Theorem 3.2, the following result turns up when considering also the space discretization and applying therefore formula (4.2):

Theorem 4.2 *Under the same hypotheses of the first part of Theorem 4.1, and assuming also that, for* $t \in [0,T]$*,* $A^l u(t) \in Z$*,* $(l = 0,1,2,3)$*, it happens that* $\rho_{n,h} = O(k^3 + k\varepsilon_h)$*. Moreover, under the additional hypotheses of the second part of Theorem 4.1, together with condition (3.12), it follows that* $A_{h,0}^{-1}\rho_{n,h} = O(k^4 + k\eta_h + k^2\varepsilon_h)$*.*

4.4 Global error of the full discretization

This subsection is different from 4.1.3 in the fact that, for both Dirichlet and Robin/Neumann boundary conditions, numerical differentiation must be used to approximate the corresponding boundary values in (4.2). Because of that, in order to assure convergence with this technique, we will have to ask that k is sufficiently small with respect to h^γ, where γ is the parameter which turns up when applying numerical differentiation in space, as stated in Subsection 4.1. Again, the classical argument would lead to a worse bound for the global error than in parabolic problems, when a summation-by-parts arguments can be used.

Theorem 4.3 *Under the hypotheses of the first part of Theorem 4.2, if there exists a constant* C *such that*

$$\frac{k}{h^\gamma} \leq C, \tag{4.4}$$

when considering Dirichlet boundary conditions, $e_{n,h} = O(k^2 + \varepsilon_h + k\nu_h)$ *and, with Robin/Neumann boundary conditions,* $e_{n,h} = O(k^2 + \varepsilon_h + k\nu_h + k\mu_{k,1})$*, where* ν_h *and* $\mu_{k,1}$ *are the errors coming respectively from numerical differentiation in space and time according to Subsection 4.1. On the other hand, under the hypotheses of the second part of Theorem 4.2, but assuming also (3.13) and that*

$$\begin{aligned} &\phi \in C^4,\ h \in C^4([0,T], D(A^2)),\ u \in C^5([0,T], D(A^3)),\\ &A^l u(t) \in Z,\ l = 0,1,2,3,\ A^l h(t) \in Z,\ l = 0,1,2, \quad t \in [0,T], \end{aligned} \tag{4.5}$$

it follows that, when considering Dirichlet boundary conditions, $e_{n,h} = O(k^3 + k\varepsilon_h + \eta_h + k\nu_h)$ *and, with Robin/Neumann boundary conditions,* $e_{n,h} = O(k^3 + k\varepsilon_h + \eta_h + k\mu_{k,1} + k\nu_h)$*.*

5 Searching for local order 4

The idea is again to calculate the stages as in (3.1) but with v_n, $w_{n,j}$ as in (4.1), and u_{n+1} through (3.3) but with $\tilde{v}_n$, $\tilde{w}_{n,j}$ satisfying

$$\begin{cases} \dot{\tilde{v}}_n(\sigma) = A\tilde{v}_n(\sigma), \\ \tilde{v}_n(0) = u_n, \\ \partial\tilde{v}_n(\sigma) = \partial[u(t_n)+\sigma Au(t_n)+\frac{\sigma^2}{2}A^2u(t_n)+\frac{\sigma^3}{6}A^3u(t_n)], \end{cases}$$

$$\begin{cases} \dot{\tilde{w}}_{n,j}(\sigma) = A\tilde{w}_{n,j}(\sigma), \\ \tilde{w}_{n,j}(0) = f(t_n+c_jk,K_{n,j}), \\ \partial\tilde{w}_{n,j}(\sigma) = \partial\Bigg[f\Bigg(t_n+c_jk,u(t_n)+c_jkAu(t_n)+\frac{c_j^2k^2}{2}A^2u(t_n) \\ \qquad +k\sum_{r=1}^{j-1}a_{j,r}[f(t_n+c_rk,u(t_n)+c_rk\dot{u}(t_n))+(c_j-c_r)kAf(t_n,u(t_n))]\Bigg) \\ \qquad +\sigma Af(t_n+c_jk,u(t_n)+c_jk\dot{u}(t_n))+\frac{s^2}{2}A^2f(t_n,u(t_n))\Bigg], \end{cases}$$

where one more order of accuracy has been considered for the boundaries with respect to (4.1). Again, after discretizing these problems in space and using the variation-of-constants formula, the following full discretization formulas arise:

$$\begin{aligned} K_{n,h,i} &= e^{c_ikA_{h,0}}U_{n,h}+\sum_{l=1}^{3}c_i^lk^l\varphi_l(c_ikA_{h,0})C_h\partial A^{l-1}u(t_n) \\ &+k\sum_{j=1}^{i-1}a_{ij}\Bigg[e^{(c_i-c_j)kA_{h,0}}f(t_n+c_jk,K_{n,h,j}) \\ &\qquad +(c_i-c_j)k\varphi_1((c_i-c_j)kA_{h,0})C_h\partial f(t_n+c_jk,u(t_n)+c_jk\dot{u}(t_n)) \\ &\qquad +(c_i-c_j)^2k^2\varphi_2((c_i-c_j)kA_{h,0})C_h\partial Af(t_n,u(t_n))\Bigg], \\ U_{n+1,h} &= e^{kA_{h,0}}U_{n,h}+\sum_{l=1}^{4}k^l\varphi_l(kA_{h,0})C_h\partial A^{l-1}u(t_n) \\ &+k\sum_{i=1}^{s}b_i\Bigg[e^{(1-c_i)kA_{h,0}}f(t_n+c_ik,K_{n,h,i}) \\ &\qquad +(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_h\partial f\Bigg(t_n+c_ik,u(t_n)+c_ikAu(t_n)+\frac{c_i^2k^2}{2}A^2u(t_n) \\ &\qquad\qquad +k\sum_{j=1}^{i-1}a_{ij}[f(t_n+c_jk,u(t_n)+c_jk\dot{u}(t_n))+(c_i-c_j)kAf(t_n,u(t_n))]\Bigg) \\ &\qquad +(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_h\partial Af(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n)) \\ &\qquad +(1-c_i)^3k^3\varphi_3((1-c_i)kA_{h,0})C_h\partial A^2f(t_n,u(t_n))\Bigg]. \end{aligned} \tag{5.1}$$

Remark 5.1 We notice that, if $\partial u(t)=\partial Au(t)=\partial A^2u(t)=\partial A^3u(t)=0$, from (2.1) it follows that $\partial f(t,u(t))=\partial Af(t,u(t))=\partial A^2f(t,u(t))=0$. As in Remark 4.1,

$\partial f(t_n+c_ik,u(t_n+c_ik))=0$ differs from $\partial f(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n))$ in $O(k^2)$. Then, the stages in (5.1) differ from those in the standard approach (2.17) in

$$k\sum_{j=1}^{i-1}a_{ij}(c_i-c_j)k\varphi_1((c_i-c_j)kA_{h,0})C_hO(k^2)=k\sum_{j=1}^{i-1}a_{ij}[e^{(c_i-c_j)kA_{h,0}}-I]A_{h,0}^{-1}C_hO(k^2)$$
$$=O(k^3).$$

On the other hand, $\partial f(t_n+c_ik,u(t_n+c_ik))=0$ also differs from the factor with the big parenthesis in (5.1) in $O(k^3)$ and $\partial Af(t_n+c_ik,u(t_n+c_ik))=0$ differs from $\partial Af(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n))$ in $O(k^2)$. Because of all this, the difference in the numerical solution between (5.1) and the standard approach is

$$k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}O(k^3)+(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_hO(k^3)$$
$$+(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_hO(k^2)\Big]$$
$$=k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}O(k^3)+[e^{(1-c_i)kA_{h,0}}-I]A_{h,0}^{-1}C_hO(k^3)$$
$$+(1-c_i)k[\varphi_1((1-c_i)kA_{h,0})-I]A_{h,0}^{-1}C_hO(k^2)\Big]=O(k^4).$$

This justifies, through Theorems 5.1 and 5.2, that the local error with the standard approach, under these particular boundary conditions, behaves with order 4 under the assumptions of those theorems.

5.1 Calculation or approximation of the boundaries which are required to achieve local order 4

Apart from the terms on the boundaries which were already necessary to achieve local order 3, now

$$\partial A^3u(t_n),\quad \partial A^2f(t_n,u(t_n)) \text{ and } \partial Af(t_n+c_ik,u(t_n)+c_ik\dot{u}(t_n)) \tag{5.2}$$

must also be calculated. Using (2.1) and simplifying notation,

$$\partial A^3u=\partial[\ddot{u}-(f_{tt}+2f_{tu}\dot{u}+f_{uu}\dot{u}^2+f_u\ddot{u})]-\partial[A(f_t+f_u\dot{u})]-\partial A^2f, \tag{5.3}$$

where here everything is assumed to be evaluated either at t_n or $(t_n,u(t_n))$. Now, in order to calculate $\partial[A(f_t+f_u\dot{u})]$ and ∂A^2f, we can see that, in case A is the second derivative in one dimension, using (2.5),

$$A(f_t+f_u\dot{u})=\phi'''(u)u_x^2\dot{u}+\phi''(u)u_{xx}\dot{u}+2\phi''(u)u_x\dot{u}_x+\phi'(u)\dot{u}_{xx}+h_{txx},$$

and it happens that u_{xx} and $\dot{u}_{xx}$ can be calculated through

$$u_{xx}=\dot{u}-\phi(u)-h,\quad \dot{u}_{xx}=\ddot{u}-\phi'(u)\dot{u}-h_t. \tag{5.4}$$

As for $A^2 f$,

$$A^2 f = \phi^{(4)}(u)u_x^4 + 6\phi^{(3)}(u)u_x^2 u_{xx} + 3\phi''(u)u_{xx}^2 + 4\phi''(u)u_x u_{xxx} + \phi'(u)u_{xxxx} + h_{xxxx},$$

where u_{xx} can be calculated as in (5.4) and

$$u_{xxx} = \dot{u}_x - \phi'(u)u_x - h_x, \quad u_{xxxx} = \ddot{u} - \phi'(u)\dot{u} - h_t - \phi''(u)u_x^2 - \phi'(u)(\dot{u} - \phi(u) - h) - h_{xx}.$$

Finally,

$$\begin{aligned} &Af(t_n + c_i k, u(t_n) + c_i k\dot{u}(t_n)) \\ &= \phi''(u + c_i k\dot{u})(u_x + c_i k\dot{u}_x)^2 + \phi'(u + c_i k\dot{u})(u_{xx} + c_i k\dot{u}_{xx}) + h_{xx}(t_n + c_i k), \end{aligned}$$

where, in the right-hand-side u and its derivatives are all evaluated at $t = t_n$ and, for u_{xx}, (5.4) can again be used.

Therefore, when A is the second derivative in space and Dirichlet boundary conditions are considered, the boundary of every term is exactly calculable in terms of data except for u_x and $\dot{u}_x$. Then, u_x can be approximated as in Subsection 4.1 and so $\dot{u}_x$ considering also space numerical differentiation over the exact values of $\dot{u}$ on the boundary and the approximated values of $\dot{u}$ in the interior of the domain, which can again be approximated by numerical differentiation in time from the values of the numerical solution. It can thus be deduced that, in this case, the approximation of $\dot{u}_x$ at the boundary differs from the exact in $O(\nu_h + \frac{e_{n,h}}{hk} + \frac{\mu_{k,1}}{h})$, where $\mu_{k,1}$ is the error which comes from the approximation of the first derivative if the values from which it is calculated were all exact. Because of this, the error of approximation of the first two terms in (5.2) behaves as $O(\nu_h + \frac{e_{n,h}}{hk} + \frac{\mu_{k,1}}{h})$ and, for the last one, as $O(\nu_h + \frac{e_{n,h}}{h} + k\frac{\mu_{k,1}}{h})$ due to the factor k multiplying $\dot{u}_x$. For a general operator A, we will assume all terms in (5.2) are calculated except for an error as that in Table 4.1 for some real value γ.

With Robin/Neumann boundary conditions, in one dimension and with A the second derivative in space, $u|_{\partial\Omega}, u_x|_{\partial\Omega}, \dot{u}|_{\partial\Omega}, \dot{u}_x|_{\partial\Omega}, \ddot{u}|_{\partial\Omega}, \ddot{u}_x|_{\partial\Omega}$ will also be needed. (Notice that $\ddot{u}$ just appears linearly in (5.3) and therefore is given directly in terms of data through $\partial\, \ddot{u} = \ddot{g}$.) Then, $u|_{\partial\Omega}$ and $u_x|_{\partial\Omega}$ are calculated except for $O(e_{n,h})$ as in Remark 3.1; $\dot{u}|_{\partial\Omega}$ and $\dot{u}_x|_{\partial\Omega}$ except for $O(\mu_{k,1} + \frac{e_{n,h}}{k})$ as in Subsection 4.1 and $\ddot{u}|_{\partial\Omega}$ and $\ddot{u}_x|_{\partial\Omega}$ in a similar way through numerical differentiation except for $O(\mu_{k,2} + \frac{e_{n,h}}{k^2})$, where $\mu_{k,2}$ comes from the error in the numerical approximation of the second derivative. For a general operator A, we thus assume that the error in the calculation of the first two boundaries of (5.2) is as written in the right-bottom part of Table 4.1 where the last two terms come from the possible error in the numerical approximation of some spatial derivatives of u and $\dot{u}$. For the boundary of the last term in (5.2), the error in the calculation, due to the factor k multiplying $\dot{u}$, is also as specified in Table 4.1.

5.2 Local error of the time semidiscretization

When discretizing in time as specified at the beginning of Subsection 5, with a similar proof to that of Theorems 3.1 and 4.1 (see [7]), the following result follows for the local error if enough regularity is assumed:

Theorem 5.1 *Assuming that*

$$\phi \in C^3,\ h \in C^3([0,T],D(A^3)),\ u \in C^4([0,T],D(A^4)), \tag{5.5}$$

and if the Runge-Kutta tableau corresponds to a method of classical order ≥ 3*, it follows that* $\rho_n = O(k^4)$*. Moreover, if* $f \in C^4([0,T]\times X,X), u \in C^5([0,T],X)$*, (3.10) holds and the Runge-Kutta tableau corresponds to a method of classical order* ≥ 4*, it follows that* $A_0^{-1}\rho_n = O(k^5)$*.*

5.3 Local error of the full discretization

In a similar way to the proof of Theorem 4.2, it follows that, when considering formulas (5.1), the local error after full discretization behaves in the following way:

Theorem 5.2 *Under the same hypotheses of the first part of Theorem 5.1, and assuming also that, for* $t \in [0,T]$*,*

$$A^l u(t) \in Z,\ l = 0,1,\ldots,4, \tag{5.6}$$

it happens that $\rho_{n,h} = O(k^4 + k\varepsilon_h)$*. Moreover, under the additional hypotheses of the second part of Theorem 5.1, together with condition (3.12),* $A_{h,0}^{-1}\rho_{n,h} = O(k^5 + k\eta_h)$*.*

5.4 Global error of the full discretization

In a similar way to Subsection 4.4, the following result follows for the global error after full discretization with (5.1):

Theorem 5.3 *Under hypotheses of the first part of Theorem 5.2 and assuming that (4.4) holds, when considering Dirichlet boundary conditions,* $e_{n,h} = O(k^3 + \varepsilon_h + k\nu_h + k\mu_{k,1})$ *and, with Robin/Neumann boundary conditions,* $e_{n,h} = O(k^3 + \varepsilon_h + k\nu_h + k\mu_{k,1} + k^2\mu_{k,2})$*, where* ν_h *and* $\mu_{k,1}, \mu_{k,2}$ *are the errors coming from numerical differentiation in space and time according to Subsection 5.1. On the other hand, under the hypotheses of the second part of Theorem 5.2, but assuming also (3.13) and that*

$$\begin{aligned} &\phi \in C^5,\ h \in C^5([0,T],D(A^3)),\ u \in C^6([0,T],D(A^4)) \\ &A^l u(t) \in Z, l = 0,1,\ldots,4, \quad A^l h(t) \in Z, l = 0,1,2,3, \quad t \in [0,T], \end{aligned} \tag{5.7}$$

it follows that, with Dirichlet boundary conditions, $e_{n,h} = O(k^4 + k\varepsilon_h + \eta_h + k\nu_h + k\mu_{k,1})$ *and, with R/N boundary conditions,* $e_{n,h} = O(k^4 + k\varepsilon_h + \eta_h + k\mu_{k,1} + k^2\mu_{k,2} + k\nu_h)$*.*

6 Numerical results

In this section, we show some numerical experiments which corroborate the previous results. For that, we have considered the following set of problems

$$\begin{aligned} u_t(t,x) &= u_{xx}(t,x) + u^2(t,x) + h(t,x), \quad x \in [0,1], \quad t \in [0,1], \\ u(0,x) &= u_0(x), \end{aligned} \tag{6.1}$$

where the boundary conditions are either Dirichlet

$$u(t,0) = g_0(t), \quad u(t,1) = g_1(t), \tag{6.2}$$

or mixed (Dirichlet/Neumann),

$$u(t,0) = g_0(t), \quad u_x(t,1) = g_1(t), \tag{6.3}$$

and where $h(t,x)$, $u_0(x)$ and $g_0(t), g_1(t)$ are such that the exact solution of the problem is

$$u(x,t) = \cos(x+t). \tag{6.4}$$

In the first place, as space discretization we have considered the symmetric 2nd-order difference scheme for which, in the Dirichlet case (6.2),

$$A_{h,0} = \text{tridiag}(1,-2,1)/h^2, \quad C_h[g_0(t),g_1(t)]^T = [g_0(t),0,\ldots,0,g_1(t)]^T/h^2, \tag{6.5}$$

and, in the Dirichlet/Neumann case (6.3),

$$A_{h,0} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \ldots & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & 0 & 2 & -2 \end{bmatrix}, \quad C_h \begin{bmatrix} g_0(t) \\ g_1(t) \end{bmatrix} = \begin{bmatrix} \frac{1}{h^2} g_0(t) \\ 0 \\ \vdots \\ 0 \\ \frac{2}{h} g_1(t) \end{bmatrix}. \tag{6.6}$$

All differential problems (6.1) with boundary conditions (6.2)-(6.3) satisfy hypotheses (A1)-(A7) with $X = C([0,1])$ and the respective space discretizations (6.5) and (6.6) satisfy hypotheses (H1)-(H2), as it was justified in [4] for $Z = C^4([0,1])$, ε_h, η_h being $O(h^2)$ for (6.5) and $\varepsilon_h = O(h)$, $\eta_h = O(h^2)$ for (6.6). Besides, the considered solution (6.4) and f are so smooth that all conditions of regularity in the paper are satisfied. Finally, (3.10) is satisfied in the Dirichlet case (6.2) because it corresponds to bound

$$2\int_0^x \int_0^\sigma \cos(\xi+t) w''(\xi) d\xi d\sigma - 2x \int_0^1 \int_0^\sigma \cos(\xi+t) w''(\xi) d\xi d\sigma,$$

whenever $w \in D(A_0)$. Integrating twice by parts, that can be seen equal to

$$\begin{aligned} 2\cos(x+t)w(x) + 4\int_0^x \sin(\sigma+t) w(\sigma) d\sigma - 2\int_0^x \int_0^\sigma \cos(\xi+t) w(\xi) d\xi d\sigma \\ -4x \int_0^1 \sin(\sigma+t) w(\sigma) d\sigma + 2x \int_0^1 \int_0^\sigma \cos(\xi+t) w(\xi) d\xi d\sigma, \end{aligned}$$

Table 6.1 Local error when integrating Dirichlet problem with non-vanishing boundary conditions with the standard approach (2.17) associated to the second-order method (6.7).

h	k=1e-3	k=5e-4	k=2.5e-4	k=1.25e-4
2e-3	1.2404e+2	6.1563e+1	3.0339e+1	1.4751e+1
1e-3	4.9902e+2	2.4903e+2	1.2404e+2	6.1563e+1
5e-4	1.9990e+3	9.9902e+2	4.9902e+2	2.4903e+2

Table 6.2 Global error when integrating Dirichlet problem with non-vanishing boundary conditions with the standard approach (2.17) associated to the second-order method (6.7).

h	k=1e-3	k=5e-4	k=2.5e-4	k=1.25e-4
2e-3	6.7023e+1	3.3264e+1	1.6394e+1	7.9729e+0
1e-3	2.6962e+2	1.3455e+2	6.7023e+1	3.3264e+1
5e-4	1.0801e+3	5.3977e+2	2.6962e+2	1.3455e+2

Table 6.3 Local and global error when integrating Dirichlet problem with nonvanishing boundary conditions with the suggested approach (3.6) associated to the second-order method (6.7), with which no numerical differentiation is required.

k	1e-03	5e-4	2.5e-4	1.25e-4
Local error	1.5664e-7	3.9176e-8	9.7933e-9	2.4473e-9
Order		2.00	2.00	2.00
Global error	8.2929e-7	2.0714e-7	5.1712e-8	1.2903e-8
Order		2.00	2.00	2.00

which can be clearly bounded by $\|w\|_\infty$. Similarly, in the Dirichlet/Neumann case, (3.10) corresponds to bound

$$
\begin{aligned}
&2\int_0^x\int_0^\sigma \cos(\xi+t)w''(\xi)d\xi d\sigma - 2x\int_0^1 \cos(\xi+t)w''(\xi)d\xi \\
&= 2\cos(x+t)w(x)+4\int_0^x \sin(\sigma+t)w(\sigma)d\sigma - 2\int_0^x\int_0^\sigma \cos(\xi+t)w(\xi)d\xi d\sigma \\
&\quad -2x\sin(t+1)w(1)+2x\int_0^1 \cos(\xi+t)w(\xi)d\xi,
\end{aligned}
$$

which is again bounded by $\|w\|_\infty$. Although we do not provide a proof for the condition (3.12) in the maximum norm, as expected from the fact that (3.10) is satisfied, it can be numerically verified that this condition holds uniformly on h for $A_{h,0}$ in (6.5) and (6.6).

6.1 Second-order method

We first show the results which are obtained when integrating problem (6.1) associated to the Dirichlet boundary conditions with the Lawson method which is con-

Table 6.4 Local and global error when integrating Dirichlet problem with nonvanishing boundary conditions with the suggested approach (4.2) associated to the second-order method (6.7), for which numerical differentiation is required.

k	8e-3	4e-3	2e-3	1e-3
Local error	1.3126e-7	1.6797e-8	2.1350e-9	2.7857e-10
Order		2.97	2.98	2.94
Global error	5.9892e-7	1.4972e-7	3.7367e-8	9.2309e-9
Order		2.00	2.00	2.02

structed with the second-order RK tableau

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \tag{6.7}$$

As Tables 6.1 and 6.2 show, when using the standard approach (2.17) for integrating (6.1), the local and global orders are 1, the errors are very big and even grow when h diminishes. However, that bad behaviour can be solved by using the suggested approach (3.6), where every term on the boundary can be calculated in terms of data, without resorting to numerical differentiation. In such a way, local and global order 2 is obtained, as shown in Table 6.3 with $h = 5 \times 10^{-4}$, for which the error in space is negligible and does not grow with h. This corroborates Theorems 3.2 and 3.3. On the other hand, with this method, it is even possible to achieve local order 3 with formula (4.2), although numerical differentiation is required to approximate the boundary of the first derivative in space of the exact solution, as it is thoroughly explained in Subsection 4.1. For that, we have considered the 2-BDF formula, for which $v_h = O(h^2)$ and, as already predicted by the first part of Theorems 4.2 and 4.3, Table 6.4 shows local order near 3 and global order 2 in time, but with a size of errors quite smaller than those of Table 6.3. (We notice that again the terms of the error which come from the space discretization and numerical differentiation are negligible compared to the error which just depends on the time stepsize k.) Moreover, condition (4.4) seems not to be very restrictive since, as stated in Subsection 4.1, $\gamma = 1$ because A corresponds to second-order differentiation in space.

Although it is not an aim of this paper to compare with other methods, we give a brief comparison in CPU time with this exponential Runge-Kutta method (suggested in [13,20]), and which also has as underlying Runge-Kutta method that in (6.7).

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & \varphi_1 & 0 \\ \hline & \varphi_1 - \varphi_2 & \varphi_2 \end{array}. \tag{6.8}$$

This method happens to show also second order for the corresponding discretization (2.16) of problem (6.1). We have implemented this method as suggested in [13], using Krylov methods for the evaluation of the exponential-type functions. More precisely, the subroutines in [18], which are the same ones which have been used for the implementation of the different techniques described above for Lawson method based on (6.7). As Figure 6.1 shows, the suggested implementation of Lawson method (4.2),

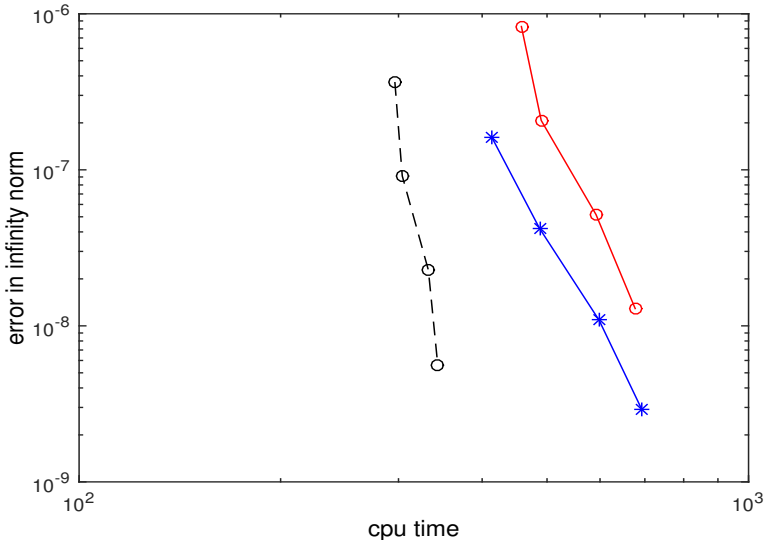

Fig. 6.1 Error against CPU time when integrating problem (6.1), using the exponential RK method (6.8) (blue asterisks), the suggested approach (3.6) for Lawson method based on (6.7) (red circles and continuous line) and the suggested approach (4.2) for Lawson method associated to (6.7) (black circles and dashed line). The parameters k and h have been chosen as for Tables 6.3 and 6.4.

Table 6.5 Local and global error when integrating mixed D/N problem with nonvanishing boundary conditions with the standard approach associated to the third-order method (6.9), $h = 10^{-3}$.

k	0.2	0.1	0.05	0.025
Local error	9.7639e-1	9.8964e-1	9.9108e-1	9.8877e-1
Order		-0.02	-0.00	0.00
Global error	5.3822e-1	5.3736e-1	5.3613e-1	5.3439e-1
Order		0.00	0.00	0.00

which avoids order reduction for both local and global errors through numerical differentiation, is more efficient than (6.8). We also notice that, for a same stepsize ($k = 10^{-3}$), approach (4.2) is cheaper than (3.6) in spite of the fact that more terms are calculated and numerical differentiation is required. An explanation for that is given in [8].

6.2 Third-order method

In this subsection we show the results which are obtained when considering (6.1) associated to the mixed Dirichlet/Neumann boundary conditions in (6.3) and inte-

Table 6.6 Local and global error when integrating mixed D/N problem with nonvanishing boundary conditions with the suggested approach (4.2) associated to the third-order method (6.9), for which numerical differentiation is required, $h = 10^{-3}$.

k	0.2	0.1	0.05	0.025
Local error	1.3911e-3	1.7489e-3	2.1806e-5	2.7212e-6
Order		2.99	3.00	3.00
Global error	1.5136e-3	2.3369e-4	2.9913e-5	3.6533e-6
Order		2.70	2.97	3.03

Table 6.7 Local and global error when integrating Dirichlet problem with nonvanishing boundary conditions with the suggested approach (5.1) associated to the fourth-order method (6.10), when the terms on the boundary are exactly provided, $h = 5 \times 10^{-4}$.

k	0.2	0.1	0.05	0.025
Local error	1.8356e-4	1.0396e-5	6.1679e-7	3.7509e-8
Order		4.14	4.08	4.04
Global error	1.9072e-4	9.3054e-6	5.4646e-7	3.5333e-8
Order		4.36	4.09	3.95

grating it in time with the Lawson method associated to the third order Heun method

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array} . \tag{6.9}$$

The standard approach shows no convergence either on the local nor the global error when the timestepsize diminishes, as it is shown in Table 6.5. (Notice the different behaviour with respect to the standard approach in Tables 6.1 and 6.2. Here the errors do not diminish with k but, although not shown here for the sake of brevity, they neither grow when h diminishes as it happens in those tables. This is due to the fact that now every c_i is different from 1 [7]). We can get local and thus global order 3 with our modified approach (4.2), by calculating the terms on the boundary following again Subsection 4.1. For the Dirichlet boundary condition, we have used numerical differentiation in space with the 2-BDF formula and, for the Neumann one, numerical differentiation in time with the 3-BDF scheme. In such a case, Theorem 4.2 as well as the second part of Theorem 4.3 apply, with $\nu_h = O(h^2)$ and $\mu_{k,1} = O(k^3)$. Therefore, when the error in space is negligible, order 3 in the time stepsize should be seen, as Table 6.6 corroborates.

Table 6.8 Local and global error when integrating Dirichlet problem with nonvanishing boundary conditions with the suggested approach (5.1) associated to the fourth-order method (6.10), when the terms on the boundary are calculated through numerical differentiation and Gauss-Lobatto collocation space discretization is used.

k	2.5e-2	1.25e-2	6.25e-3	3.125e-3
Local error	3.4537e-8	2.0441e-9	1.1954e-10	6.8247e-12
Order		4.08	4.10	4.13
Global error	3.3314e-8	2.0054e-9	1.1968e-10	7.0050e-12
Order		4.05	4.07	4.09

6.3 Fourth-order method

Finally, we show that local and global order 4 can be obtained when integrating in time with the Lawson method associated to the fourth-order RK method

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{3} & \frac{1}{3} & & & \\ \frac{2}{3} & -\frac{1}{3} & 1 & & \\ 1 & 1 & -1 & 1 & \\ \hline & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} \end{array} . \tag{6.10}$$

Nevertheless, we point out that condition (4.4) is in fact necessary. We remind that, in our problem (6.1), $\gamma = 1$, as it was justified in Subsections 4.1 and 5.1. For the sake of brevity, we will center on the Dirichlet boundary condition in (6.2), and we will directly integrate that problem with the suggested formulas (5.1) by inserting the needed boundaries in an exact way from the known solution. As Table 6.7 shows, local and global order 4 are observed in that way. However, when not knowing the exact solution, those boundaries must be calculated in terms of data following Subsection 5.1. For that, we have considered again the 3 (resp. 2)-BDF formula for the numerical differentiation in time (resp. in space) and, according to Theorems 5.2 and 5.3, global order 4 in the time stepsize should be observed when the error in space is negligible and (4.4) holds for some constant C. However, as the error in space is just of second order, in order that the error in space is negligible with respect to that in time, h must be quite small with respect to k, and then the global error explodes to infinity with the parameters of Table 6.7 because condition (4.4) is not satisfied for a suitable constant C.

In spite of all this, the problem can be solved by considering a more accurate space discretization. Thus we have considered a Gauss-Lobatto collocation space discretization with 17 nodes, for which the error in space is nearly of the order of rounding errors for this problem. Besides, the space grid is quite moderate, so condition (4.4) is very weak in this case. Considering then numerical differentiation in time as before and numerical differentiation in space through the derivation of the corresponding collocation polynomials, the results in Table 6.8 are obtained, where both local and global order 4 are achieved.

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7 Appendix

7.1 Proof of Theorem 3.1

Using Lemma 3.1 in [3],

$$\begin{aligned}
\bar{v}_n(s) &= u(t_n) + s\varphi_1(sA_0)Au(t_n), \qquad (7.1)\\
\bar{\bar{v}}(s) &= u(t_n) + sAu(t_n) + s^2\varphi_2(sA_0)A^2u(t_n),\\
\bar{w}_{n,i}(s) &= e^{sA_0}f(t_n + c_ik, \bar{K}_{n,i}),\\
\bar{\bar{w}}_{n,i}(s) &= e^{sA_0}[f(t_n + c_ik, \bar{K}_{n,i}) - f(t_n, u(t_n))] + f(t_n, u(t_n))\\
&\quad + s\varphi_1(sA_0)Af(t_n, u(t_n)).
\end{aligned}$$

Then,

$$\begin{aligned}
\bar{K}_{n,i} &= u(t_n) + c_ik\varphi_1(c_ikA_0)Au(t_n) + k\sum_{j=1}^{i-1} a_{ij}e^{(c_i-c_j)kA_0}f(t_n + c_jk, \bar{K}_{n,j}) \qquad (7.2)\\
&= u(t_n) + O(k), \qquad i = 1, \dots, s, \qquad (7.3)\\
\bar{u}_{n+1} &= u(t_n) + kAu(t_n) + k^2\varphi_2(kA_0)A^2u(t_n)\\
&\quad + k\sum_{i=1}^{s} b_i\Big[e^{(1-c_i)kA_0}[f(t_n + c_ik, \bar{K}_{n,i}) - f(t_n, u(t_n))] + f(t_n, u(t_n))\\
&\qquad + (1-c_i)k\varphi_1((1-c_i)kA_0)Af(t_n, u(t_n))\Big] \qquad (7.4)\\
&= u(t_n) + k[Au(t_n) + f(t_n, u(t_n))] + O(k^2) = u(t_n) + k\dot{u}(t_n) + O(k^2),
\end{aligned}$$

where, for the last line, (3.9), (A4) together with (7.3) and the first condition of (2.11) have been used. From this, the first result on the local error follows.

As for the second result, looking at the term in k^2 in $\bar{u}_{n+1}$ and using that $u \in C^3([0,T],X)$, we can notice that

$$\begin{aligned}
A_0^{-1}\rho_{n+1} &= k^3(kA_0)^{-1}(\varphi_2(kA_0) - \frac{1}{2}I)A^2u(t_n) + \frac{k^2}{2}A_0^{-1}A^2u(t_n)\\
&\quad + k^2\sum_{i=1}^{s} b_i(1-c_i)((1-c_i)kA_0)^{-1}[e^{(1-c_i)kA_0} - I][f(t_n + c_ik, \bar{K}_{n,i}) - f(t_n, u(t_n))]\\
&\quad + k\sum_{i=1}^{s} b_iA_0^{-1}[f(t_n + c_ik, \bar{K}_{n,i}) - f(t_n, u(t_n))] \qquad (7.5)\\
&\quad + k^3\sum_{i=1}^{s} b_i(1-c_i)^2((1-c_i)kA_0)^{-1}(\varphi_1((1-c_i)kA_0) - I)Af(t_n, u(t_n))\\
&\quad + k^2\sum_{i=1}^{s} b_i(1-c_i)A_0^{-1}Af(t_n, u(t_n)) - \frac{k^2}{2}\ddot{u}(t_n) + O(k^3).
\end{aligned}$$

Using (2.7), (7.3), (A4) and (3.9), the first, third and fifth terms are $O(k^3)$. As for the fourth one, considering (7.2), it can be written as

$$
\begin{aligned}
&k^2\sum_{i=1}^{s} b_i A_0^{-1} f_u(t_n,u(t_n))[c_i\varphi_1(c_i kA_0)Au(t_n)+\sum_{j=1}^{i-1} a_{ij}e^{(c_i-c_j)kA_0}f(t_n+c_jk,\bar{K}_{n,j})]\\
&\quad +k^2\sum_{i=1}^{s} b_i c_i A_0^{-1} f_t(t_n,u(t_n))+O(k^3)\\
&=k^3\sum_{i=1}^{s} b_i A_0^{-1} f_u(t_n,u(t_n))A_0 c_i (kA_0)^{-1}[\varphi_1(c_i kA_0)-I]Au(t_n)\\
&\quad +k^2(\sum_{i=1}^{s} b_i c_i)A_0^{-1} f_u(t_n,u(t_n))Au(t_n)\\
&\quad +k^3\sum_{i=1}^{s} b_i \sum_{j=1}^{i-1} a_{ij}A_0^{-1} f_u(t_n,u(t_n))A_0(kA_0)^{-1}[e^{(c_i-c_j)kA_0}-I]f(t_n,u(t_n))\\
&\quad +k^2\sum_{i=1}^{s} b_i \sum_{j=1}^{i-1} a_{ij}A_0^{-1} f_u(t_n,u(t_n))f(t_n,u(t_n))\\
&\quad +k^2\sum_{i=1}^{s} b_i c_i A_0^{-1} f_t(t_n,u(t_n))+O(k^3)\\
&=\frac{k^2}{2}A_0^{-1}[f_u(t_n,u(t_n))\dot{u}(t_n)+f_t(t_n,u(t_n))]+O(k^3),
\end{aligned}
$$

where, for the last equality, we have used (2.7) again, (3.10), the second condition in (2.11) and the fact that $\sum_{i=1}^{s} b_i c_i = 1/2$ due to the second order of the Butcher tableau. Inserting this in (7.5) and simplifying notation,

$$A_0^{-1}\rho_{n+1}=\frac{k^2}{2}A_0^{-1}[A^2u+f_u\dot{u}+f_t+Af-\ddot{u}]+O(k^3)=O(k^3),$$

where the differentiation of (2.1) with respect to time shows that the term in bracket in the previous expression vanishes.

7.2 Proof of Theorem 3.3

Firstly notice that

$$e_{n+1,h}=[U_{n+1,h}-\bar{U}_{n+1,h}]+\rho_{n+1,h}. \tag{7.6}$$

Then, using (3.6), when considering Dirichlet boundary conditions, in which case $\partial Au(t_n)$ and $\partial f(t_n,u(t_n))$ are calculated exactly in terms of data, as $\bar{U}_{n+1,h}$ is the same as $U_{n+1,h}$ but starting from $P_h u(t_n)$ instead of $U_{n,h}$,

$$
\begin{aligned}
U_{n+1,h}-\bar{U}_{n+1,h}&=e^{kA_{h,0}}[U_{n,h}-P_h u(t_n)]\\
&\quad +k\sum_{i=1}^{s} b_i e^{(1-c_i)kA_{h,0}}[f(t_n+c_ik,K_{n,h,i})-f(t_n+c_ik,\bar{K}_{n,h,i})],
\end{aligned}
\tag{7.7}
$$

where, recursively, for $i = 1, \dots, s$,

$$K_{n+1,h,i} - \bar{K}_{n+1,h,i} = e^{c_i k A_{h,0}}[U_{n,h} - P_h u(t_n)] + k \sum_{j=1}^{i-1} a_{ij} e^{(c_i - c_j) k A_{h,0}} [f(t_n + c_j k, K_{n,h,j}) - f(t_n + c_j k, \bar{K}_{n,h,j})]. \tag{7.8}$$

In such a way, it is inductively proved that $K_{n+1,h,i} - \bar{K}_{n+1,h,i} = O(e_{n,h})$ and finally, using (7.7) and (7.6),

$$e_{n+1,h} = e^{k A_{h,0}} e_{n,h} + O(k e_{n,h}) + \rho_{n+1,h}, \tag{7.9}$$

from what the result follows from Theorem 3.2 by a summation-by-parts argument and a discrete Gronwall lemma in the same way than the proof of Theorem 22 in [4] for Strang method.

On the other hand, when considering Robin/Neumann boundary conditions, as, according to Remark 3.1, $\partial f(t_n, u(t_n))$ is just calculated approximately with an error which is $O(e_{n,h})$, using (3.6) again,

$$U_{n+1,h} - \bar{U}_{n+1,h} = e^{k A_{h,0}} e_{n,h} + k^2 \varphi_2(k A_{h,0}) C_h O(e_{n,h}) + k \sum_{i=1}^{s} b_i \Big[e^{(1-c_i) k A_{h,0}} [f(t_n + c_i k, K_{n,h,i}) - f(t_n + c_i k, \bar{K}_{n,h,i})] + (1 - c_i) k \varphi_1((1 - c_i) k A_{h,0}) C_h O(e_{n,h}) \Big],$$

where $K_{n+1,h,i} - \bar{K}_{n+1,h,i}$ is the same as in (7.8) because $\partial u(t_n)$ is given exactly in terms of data with this type of boundary conditions. Then, using (2.7),

$$U_{n+1,h} - \bar{U}_{n+1,h} = e^{k A_{h,0}} e_{n,h} + k[\varphi_1(k A_{h,0}) - I] A_{h,0}^{-1} C_h O(e_{n,h}) + k \sum_{i=1}^{s} b_i \Big[e^{(1-c_i) k A_{h,0}} O(e_{n,h}) + [e^{(1-c_i) k A_{h,0}} - I] A_{h,0}^{-1} C_h O(e_{n,h}) \Big].$$

Using now (H2c), it follows that $U_{n+1,h} - \bar{U}_{n+1,h} = e^{k A_{h,0}} e_{n,h} + O(k e_{n,h})$, from what (7.9) applies again and the result follows in the same way as above.

7.3 Proof of Theorem 4.3

For the proof, as in Theorem 3.3, we must consider the decomposition (7.6) where $\bar{U}_{n+1,h}$ is calculated as $U_{n+1,h}$ but starting from $P_h u(t_n)$ and calculating the boundaries in (4.2) in an exact way. In contrast, according to Table 4.1, when considering $U_{n+1,h}$, the boundaries in (4.2) can just be calculated approximately.

More precisely, with Dirichlet boundary conditions, the terms on the boundary for the stages in (4.2) can be calculated exactly. However, when calculating $U_{n+1,h}$,

$\partial A^2 u(t_n)$ and $\partial A f(t_n,u(t_n))$ can just be calculated except for $O(\nu_h+\frac{e_{n,h}}{h^\gamma})$. Because of this,

$$\begin{aligned}U_{n+1,h}-\bar{U}_{n+1,h} &= e^{kA_{h,0}}e_{n,h}+k^3\varphi_3(kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma})\\ &\quad +k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}[f(t_n+c_ik,K_{n,h,i})-f(t_n+c_ik,\bar{K}_{n,h,i})]\\ &\qquad +(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma})\Big],\end{aligned}$$

where $K_{n,h,i}-\bar{K}_{n,h,i}=O(e_{n,h})$ as in the proof of Theorem 3.3. Therefore, using (2.7) and (H2c),

$$\begin{aligned}U_{n+1,h}-\bar{U}_{n+1,h} &= e^{kA_{h,0}}e_{n,h}+k^2(\varphi_2(kA_{h,0})-\frac{1}{2}I)O(\nu_h+\frac{e_{n,h}}{h^\gamma})+O(ke_{n,h})\\ &\quad +k^2\sum_{i=1}^{s}b_i(1-c_i)(\varphi_1(kA_{h,0})-I)O(\nu_h+\frac{e_{n,h}}{h^\gamma}),\end{aligned}$$

from what, using condition (4.4),

$$e_{n+1,h}=e^{kA_{h,0}}e_{n,h}+O(ke_{n,h})+O(k^2\nu_h)+\rho_{n+1,h}.$$

The classical argument of convergence and the first part of Theorem 4.2 leads then to the first result of this theorem for Dirichlet boundary conditions. For the second part, the second part of Theorem 4.2 must be used, apart from (3.13) and the additional regularity (4.5).

On the other hand, with Robin/Neumann boundary conditions, there is some error when approximating the boundaries for both the stages and the numerical solution. More precisely, using Table 4.1 and (4.2),

$$\begin{aligned}K_{n,h,i}-\bar{K}_{n,h,i} &= e^{c_ikA_{h,0}}e_{n,h}+c_i^2k^2\varphi_2(c_ikA_{h,0})C_hO(e_{n,h})\\ &\quad +k\sum_{j=1}^{i-1}a_{ij}[O(e_{n,h})+(c_i-c_j)k\varphi_1((c_i-c_j)kA_{h,0})C_hO(e_{n,h})]\\ &= e^{c_ikA_{h,0}}e_{n,h}+c_ik[\varphi_1(c_ikA_{h,0})-I]O(e_{n,h})\\ &\quad +k\sum_{j=1}^{i-1}a_{ij}\Big[O(e_{n,h})+[e^{(c_i-c_j)kA_{h,0}}-I]O(e_{n,h})\Big]\\ &= e^{c_ikA_{h,0}}e_{n,h}+O(ke_{n,h})=O(e_{n,h}),\end{aligned}$$

and then

$$\begin{aligned}
U_{n+1,h}-\bar{U}_{n+1,h} &= e^{kA_{h,0}}e_{n,h}+k^3\varphi_3(kA_{h,0})C_hO(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\\
&\quad +k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}[f(t_n+c_ik,K_{n,h,i})-f(t_n+c_ik,\bar{K}_{n,h,i})]\\
&\qquad +(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_hO(k\mu_{k,1}+e_{n,h})\\
&\qquad +(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_hO(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\Big]\\
&= e^{kA_{h,0}}e_{n,h}+k^2[\varphi_2(kA_{h,0})-\frac{1}{2}I]O(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\\
&\quad +k\sum_{i=1}^{s}b_i\Big[O(e_{n,h})+[e^{(1-c_i)kA_{h,0}}-I]O(k\mu_{k,1}+e_{n,h})\\
&\qquad +(1-c_i)k[\varphi_1(kA_{h,0})-I]O(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\Big].
\end{aligned}$$

From this, under condition (4.4),

$$e_{n+1,h}=e^{kA_{h,0}}e_{n,h}+O(ke_{n,h}+k^2\mu_{k,1}+k^2\nu_h)+\rho_{n+1,h},$$

so that, using the first part of Theorem 4.2 and the classical argument of convergence, $e_{n,h}=O(k^2+\varepsilon_h+k\nu_h+k\mu_{k,1})$. Again, under the second set of hypotheses in Theorem 4.2 and using (3.13) and the regularity (4.5), the finer result $e_{n,h}=O(k^3+k\varepsilon_h+\eta_h+k\mu_{k,1}+k\nu_h)$ can be achieved.

7.4 Proof of Theorem 5.3

As in the proof of Theorem 4.3, we must consider the decomposition (7.6) and then study the difference $U_{h,n+1}-\bar{U}_{n+1}$ taking into account that the boundaries for $U_{h,n+1}$ in (5.1) are just calculated approximately with an error which is given through Table 4.1.

More precisely, with Dirichlet boundary conditions,

$$\begin{aligned}
U_{n+1,h}-\bar{U}_{n+1,h} &= e^{kA_{h,0}}e_{n,h}+k^3\varphi_3(kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma})\\
&\quad +k^4\varphi_4(kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma k}+\frac{\mu_{k,1}}{h^\gamma})\\
&\quad +k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}[f(t_n+c_ik,K_{n,h,i})-f(t_n+c_ik,\bar{K}_{n,h,i})]\\
&\quad +(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_hO(k^2\nu_h+k^2\frac{e_{n,h}}{h^\gamma})\\
&\quad +(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma}+\frac{k\mu_{k,1}}{h^\gamma})\\
&\quad +(1-c_i)^3k^3\varphi_3((1-c_i)kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma k}+\frac{\mu_{k,1}}{h^\gamma})\Big], \quad (7.10)
\end{aligned}$$

where

$$\begin{aligned}K_{n,h,i}-\bar{K}_{n,h,i} &= e^{c_i kA_{h,0}}e_{n,h}+c_i^3k^3\varphi_3(kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma})\\ &\quad +k\sum_{j=1}^{i-1}a_{ij}\Big[e^{(c_i-c_j)kA_{h,0}}[f(t_n+c_jk,K_{n,h,j})-f(t_n+c_jk,\bar{K}_{n,h,j})]\\ &\qquad +(c_i-c_j)^2k^2\varphi_2((c_i-c_j)kA_{h,0})C_hO(\nu_h+\frac{e_{n,h}}{h^\gamma})\Big]\\ &= O(e_{n,h}+k^2\nu_h),\end{aligned}$$

and, for the last equality, (2.7), (H2c) and (4.4) have been used. Inserting this in (7.10) and using again (2.7), (H2c) and (4.4), it follows that

$$U_{n+1,h}-\bar{U}_{n+1,h}=e^{kA_{h,0}}e_{n,h}+O(k^2\nu_h+ke_{n,h}+k^2\mu_{k,1}).$$

From here,

$$e_{n+1,h}=e^{kA_{h,0}}e_{n,h}+O(ke_{n,h})+O(k^2\nu_h+k^2\mu_{k,1})+\rho_{n+1,h},$$

and using a discrete Gronwall Lemma and the first part of Theorem 5.2, the first part of the theorem follows for Dirichlet boundary conditions. For the second part, the second part of Theorem 5.2 must be used, apart from (3.13) and the additional regularity (5.7).

As for Robin/Neumann boundary conditions, with similar arguments,

$$\begin{aligned}&K_{n,h,i}-\bar{K}_{n,h,i}\\ &= e^{c_i kA_{h,0}}e_{n,h}+c_i^2k^2\varphi_2(kA_{h,0})C_hO(e_{n,h})+c_i^3k^3\varphi_3(kA_{h,0})C_hO(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\\ &\quad +k\sum_{j=1}^{i-1}a_{ij}\Big[e^{(c_i-c_j)kA_{h,0}}[f(t_n+c_jk,K_{n,h,j})-f(t_n+c_jk,\bar{K}_{n,h,j})]\\ &\qquad +(c_i-c_j)k\varphi_1((c_i-c_j)kA_{h,0})C_hO(e_{n,h}+k(\mu_{k,1}+\frac{e_{n,h}}{k}))\\ &\qquad +(c_i-c_j)^2k^2\varphi_2((c_i-c_j)kA_{h,0})C_hO(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\Big]\\ &= e^{c_i kA_{h,0}}e_{n,h}+O(ke_{n,h}+k^2\mu_{k,1}+k^2\nu_h)=O(e_{n,h}+k^2\mu_{k,1}+k^2\nu_h),\end{aligned}$$

from what

$$
\begin{aligned}
&U_{n+1,h}-\bar{U}_{n+1,h}\\
&=e^{kA_{h,0}}e_{n,h}+k^2\varphi_2(kA_{h,0})C_hO(e_{n,h})+k^3\varphi_3(kA_{h,0})C_hO(\mu_{k,1}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\\
&\quad+k^4\varphi_4(kA_{h,0})C_hO(\mu_{k,1}+\mu_{k,2}+\frac{e_{n,h}}{k^2}+\nu_h+\frac{e_{n,h}}{kh^\gamma})\\
&\quad+k\sum_{i=1}^{s}b_i\Big[e^{(1-c_i)kA_{h,0}}[f(t_n+c_ik,K_{n,h,i})-f(t_n+c_ik,\bar{K}_{n,h,i})]\\
&\qquad\qquad+(1-c_i)k\varphi_1((1-c_i)kA_{h,0})C_hO(ke_{n,h}+k^2\mu_{k,1}+k^2\mu_{k,2}+k^2\nu_h+\frac{k^2}{h^\gamma}e_{n,h})\\
&\qquad\qquad+(1-c_i)^2k^2\varphi_2((1-c_i)kA_{h,0})C_hO(k\mu_{k,1}+k\mu_{k,2}+\frac{e_{n,h}}{k}+\nu_h+\frac{e_{n,h}}{h^\gamma})\\
&\qquad\qquad+(1-c_i)^3k^3\varphi_3((1-c_i)kA_{h,0})C_hO(\mu_{k,1}+\mu_{k,2}+\frac{e_{n,h}}{k^2}+\nu_h+\frac{e_{n,h}}{kh^\gamma})\Big]\\
&=e^{kA_{h,0}}e_{n,h}+O(ke_{n,h}+k^2\mu_{k,1}+k^3\mu_{k,2}+k^2\nu_h).
\end{aligned}
$$

From this,

$$e_{n+1,h}=e^{kA_{h,0}}e_{n,h}+O(ke_{n,h}+k^2\mu_{k,1}+k^3\mu_{k,2}+k^2\nu_h)+\rho_{n+1,h},$$

so that, using the first part of Theorem 5.2 and the classical argument of convergence, $e_{n,h}=O(k^3+\varepsilon_h+k\nu_h+k\mu_{k,1}+k^2\mu_{k,2})$. Again, under the second set of hypotheses in Theorem 5.2 and using (3.13) and the regularity (5.7), the finer result $e_{n,h}=O(k^4+k\varepsilon_h+\eta_h+k\mu_{k,1}+k^2\mu_{k,2}+k\nu_h)$ is achieved.