Analysis of order reduction when integrating linear initial boundary value problems with Lawson methods

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Abstract

In this paper, we offer a thorough analysis of the order which is observed when integrating evolutionary linear partial differential equations with Lawson methods. The analysis is performed under the general framework of C_0-semigroups in Banach spaces and though it can be applied to the numerical time integration of many initial boundary value problems which are described by linear partial differential equations. Conditions of regularity and annihilation at the boundary of these problems are then stated to justify the precise order which is observed, including fractional order of convergence.

Key words: order reduction, Lawson methods, C_0-semigroups, exponential methods.

1 Introduction

Exponential methods have very much been developed and analysed in the literature in order to integrate partial differential equations [**?**,**?**]. As the system which arises after space discretization is stiff, exponential methods are a valuable tool because they are able to integrate it in an explicit and stable way.

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[1] This research has been supported by project MTM2015-66837-P, Ministerio de Economía y Competitividad (Spain)

In this paper, we will concentrate on Lawson exponential methods. They were deduced in [?] by considering a change of variables which converts the stiff system into a non-stiff one to which a Runge-Kutta method is applied. Lawson method is then obtained by undoing the corresponding change of variables. In spite of the fact that this special type of exponential methods is one of the oldest, a thorough error analysis for it has not been performed in the literature until now because it does not satisfy some simplifying conditions which lead directly to (at least) stiff order 1 in explicit exponential methods [?]. Those conditions imply the conservation of equilibria of autonomous problems but the fact that they are not satisfied does not mean that they are not valuable methods, as it has already been proved in the literature [?,?,?]. The aim of this manuscript is to perform an analysis of the error when integrating linear problems, for which these methods can be seen as exponential quadrature rules. We will justify when order reduction is shown and when it is not. That will depend on regularity of the solution and conditions of annihilation or periodicity at the boundary. Moreover, when there is order reduction, we will explain here the precise order which is observed and, in another paper [?], we give a technique to avoid it. As this technique is very cheap, Lawson methods become a very valuable tool to integrate linear initial boundary value problems because they are able to integrate them accurately in an explicit and stable way without requiring any conditions on the coefficients of the method which could increase the computational cost, as is the case with other exponential Runge-Kutta methods in the literature until now [?,?].

The analysis will be performed with an abstract formulation of the problem, under the general framework of C_0-semigroups in Banach spaces. More precisely, we will consider the well-posed linear abstract initial value problem

$$\begin{aligned} u'(t) &= Lu(t) + f(t), \quad 0 < t < T, \\ u(0) &= u_0, \end{aligned} \tag{1}$$

where u_0 and $f(t)$ ($t \in [0,T]$) belong to a Banach space X and $L : D(L) \subset X \to X$ is a linear operator which is the infinitesimal generator of a C_0-semigroup $\{e^{tL}\}_{t\geq 0}$; so that, for certain constants $M > 0$, $\omega \in \mathbb{R}$, we have

$$\|e^{tL}\| \leq Me^{\omega t}. \tag{2}$$

For the sake of simplicity, we suppose that $\omega < 0$. As a consequence, the operator L is invertible and L^{-1} is bounded. For $\nu \geq 0$, we denote $X_\nu = D((-L)^\nu)$, endowed with the norm $\|x\|_\nu = \|(-L)^\nu x\|$, for each $x \in X_\nu$. We remark that the operators $(-L)^{-\nu}$ are bounded [?]. The use of these powers is useful to prove fractional orders of convergence. To obtain this fractional order, and to use a summation-by-parts argument for the global error, we need additional assumptions on the operator L. As for boundary conditions, homogeneous Dirichlet, Neumann and Robin conditions can be considered and they will be implicitly satisfied by all functions in $D(L)$. As we will see in Section 3, time regularity of the solution is not sufficient to obtain the classical order of the numerical integration; the order observed depends on the fact that u and some of its time derivatives belong to the domain of a certain power of L and therefore that means more conditions of annihilation at the boundary which are not natural for the solution of (1).

The case of a pure initial value problem or periodic boundary conditions can also be studied under this framework. Notice that here belonging to the domain of a certain power of L just means more regularity in space but no additional artificial conditions on the boundary. Therefore, for initial periodic boundary value problems, no order reduction is shown if the solution is regular enough in space and time.

We structure the paper as follows. In Section 2, we study sufficient conditions on the data of the problem (1) (u_0 and f) in order to assure a certain regularity of the solution u. In Section 3, we offer a thorough analysis of the local and global errors which are observed under certain assumptions on that exact solution. Finally, in Section 4, we corroborate these results when we apply Lawson methods to integrate in time some problems in 1 and 2 dimensions.

2 On the regularity of the solution

In this section, we firstly state Lemma 2.1 and Proposition 2.2, whose proof can be easily deduced from Theorem 2.4 and Corollary 2.5 in Section 4.1 of [?].

Lemma 2.1 *Let L be the infinitesimal generator of a C_0 semigroup e^{tL}. If $f \in C^1([0,T],X)$, then $\int_0^t e^{sL} f(t-s)ds \in D(L)$ and*

$$L \int_0^t e^{sL} f(t-s)ds = e^{tL} f(0) - f(t) + \int_0^t e^{sL} f'(t-s)ds.$$

Proposition 2.2 *Let L be the infinitesimal generator of a C_0 semigroup e^{tL}. If $u_0 \in D(L)$ and $f \in C^1([0,T],X)$, the unique solution u of the initial value problem (1) belongs to $C^1([0,T],X) \cap C([0,T],D(L))$ and is given by*

$$u(t) = e^{tL} u_0 + \int_0^t e^{sL} f(t-s)ds. \qquad (3)$$

Besides, its derivative is given by

$$u'(t) = e^{tL}Lu_0 + e^{tL}f(0) + \int_0^t e^{sL}f'(t-s)ds. \tag{4}$$

Now, we can obtain more regularity with a recursive argument.

Theorem 2.3 *Let $q \geq 1$ be an integer number and let L be the infinitesimal generator of a C_0 semigroup e^{tL}.*

Assume that $f \in C^q([0,T],X)$, $v_0 = u_0 \in D(L)$ and, for $1 \leq j \leq q-1$,

$$v_j = Lv_{j-1} + f^{(j-1)}(0) \in D(L). \tag{5}$$

Then, the unique solution of the initial value problem (1) belongs to $C^q([0,T],X) \cap C([0,T],D(L))$ and is given by

$$u(t) = e^{tL}u_0 + \int_0^t e^{sL}f(t-s)ds.$$

Moreover, for $0 \leq j \leq q$,

$$u^{(j)}(t) = e^{tL}v_j + \int_0^t e^{sL}f^{(j)}(t-s)ds. \tag{6}$$

With the previous proposition, we have shown conditions under which it is possible to obtain a solution of (1) which is regular enough in time without adding boundary conditions for the data u_0 and f in a separate way except for $u_0 \in D(L)$. Notice that in many problems belonging to $D(L)$ implies vanishing boundary conditions and (5) are just compatibility conditions on the data in order to assure that $u^{(q-1)}(0)$ exists and belongs to $D(L)$. However, this is not enough to obtain convergence of high order for the time discretization with Lawson methods. We now obtain the suitable regularity properties of the solution by imposing more conditions on the data of the problem, which in general are not satisfied by the solution of (1). More precisely,

Theorem 2.4 *Let L be the infinitesimal generator of a C_0 semigroup e^{tL}. Let $q \geq 1$ an integer number. Assume that*

(a) $u_0 \in D(L^q)$, $f \in C^q([0,T],X)$,

(b) *For all* $1 \le j \le q-1$ *and* $0 \le m \le j-1$, $f^{(j-1-m)}(t) \in D(L^{m+1})$ *for each* $t \in [0,T]$ *and* $L^{m+1} f^{(j-1-m)} \in C^1([0,T],X)$.

Then, the unique solution of the initial value problem (1) is given by

$$u(t) = e^{tL}u_0 + \int_0^t e^{(t-s)L} f(s)ds,$$

and satisfies that

(i) $u \in C^q([0,T],X)$.

(ii) *For all* $0 \le r \le q$ *and* $0 \le j \le r$, $u^{(j)}(t) \in D(L^{r-j})$ *for each* $t \in [0,T]$ *and*

$$L^{r-j}u^{(j)} \in C([0,T],X). \tag{7}$$

(iii) *For* $1 \le j \le q$, $u^{(j)}(t) = L^j u(t) + L^{j-1}f(t) + \ldots + f^{(j-1)}(t)$.

Proof. Assumptions (a) and (b) imply that $u_0 \in D(L)$ and that for $1 \le j \le q-1$,

$$v_j = Lv_{j-1} + f^{(j-1)}(0) = L^j u_0 + \sum_{m=0}^{j-1} L^m f^{(j-1-m)}(0) \in D(L). \tag{8}$$

Therefore, Theorem 2.3 can be applied and expression (6) can now be written in the form

$$u^{(j)}(t) = e^{tL}\left(L^j u_0 + \sum_{m=0}^{j-1} L^m f^{(j-1-m)}(0)\right) + \int_0^t e^{sL} f^{(j)}(t-s)ds. \tag{9}$$

In such a way, (ii) is proved for $j = r$ (which for $r = q$ implies (i)) and, for $j < r$, because of assumptions (a) and (b), L^{r-j} can be written before the first term in (9) and L^{r-j-1} before the derivative of f in the last one. Therefore,

$$\begin{aligned} L^{r-j}u^{(j)}(t) &= e^{tL}(L^r u_0 + \sum_{m=0}^{j-1} L^{m+r-j} f^{(j-1-m)}(0)) + L(\int_0^t e^{sL} L^{r-j-1} f^{(j)}(t-s)ds) \\ &= e^{tL}(L^r u_0 + \sum_{m=0}^{j-1} L^{m+r-j} f^{(j-1-m)}(0)) + e^{tL}L^{r-j-1}f^{(j)}(0) - L^{r-j-1}f^{(j)}(t) \\ &\quad + \int_0^t e^{sL} \frac{d}{dt}(L^{r-j-1} f^{(j)}(t-s))ds, \end{aligned}$$

where, for the last equality, Lemma 2.1 has been used with f substituted by $L^{r-j-1}f^{(j)}$. By using again assumption (b), $\frac{d}{dt}(L^{r-j-1}f^{(j)}) \in C([0,T],X)$ and therefore all the previous expression belongs to $C([0,T],X)$ and (ii) is completely proved.

Finally, (iii) just follows from an induction argument applied to (1) taking into account that all terms can be calculated because of the above. □

We have obtained in this way the time and space regularity of the solution of (1) which allows to deduce good results about the consistency and convergence of Lawson methods. This regularity can be deduced by only checking assumptions (a) and (b) on the data, initial condition and source term, of problem (1).

However, when (1) is the abstract version of an initial boundary value problem, the elements of $D(L)$ are functions which are smooth enough and satisfy suitable vanishing boundary conditions. For example, in Section 4, we consider the heat equation with Dirichlet boundary conditions, and we have $D(L) = H^2(\Omega) \cap H_0^1(\Omega)$. Therefore, assumptions (a) and (b) in Theorem 2.4 imply, when q is large, vanishing boundary conditions which are not necessarily satisfied.

3 Time discretization

We consider the time discretization of (1) by means of a Lawson method [?]. Therefore, the numerical approximation u_n at $t_n = nk$, where k is the timestepsize, is given through the recursive formula

$$u_{n+1} = e^{kL}u_n + k\sum_{i=1}^{s} b_i e^{(1-c_i)kL} f(t_n + c_i k).$$

Here, $\{b_i\}, \{c_i\}$ $(i = 1, \ldots, s)$ are the coefficients of the corresponding Runge-Kutta underlying method. Notice that for the linear problem (1), these methods just correspond to a quadrature rule approximation of the integral in (3) when $t = k$ and $u(0) = u_n$, which can also be written as

$$u(k) = e^{kL}u_n + \int_0^k e^{(k-s)L} f(t_n + s)ds.$$

Notice that when the method has classical order p for linear problems, the corresponding quadrature rule exactly integrates all polynomials of degree $\leq p-1$.

As usual, we define the local error by

$$\delta_{n,k} = u(t_{n+1}) - (e^{kL}u(t_n) + k\sum_{i=1}^{s} b_i e^{(1-c_i)kL} f(t_n + c_i k)). \tag{10}$$

Before studying how it behaves when k decreases, let us consider the following lemma.

Lemma 3.1 *Let $q \geq 1$ be an integer number and assume that, for all $0 \leq r \leq q$ and $0 \leq j \leq r$, $u^{(j)}(t) \in D(L^{r-j})$ for each $t \in [0,T]$ and (7) is satisfied. Then, the function*

$$v_{k,t_n}(t) = e^{(k-t)L}u(t_n + t) \tag{11}$$

satisfies that

$$L^{r-j}v_{k,t_n}^{(j)} \in C([0,k], X), \quad 0 \leq j \leq r, \quad 0 \leq r \leq q. \tag{12}$$

Moreover,

$$v'_{k,t_n}(t) = e^{(k-t)L}f(t_n + t). \tag{13}$$

Proof. We will prove it by induction. Notice that, for $q = 1$, because of the assumptions,

$$\begin{aligned} v'_{k,t_n}(t) &= -e^{(k-t)L}Lu(t_n + t) + e^{(k-t)L}u'(t_n + t), \\ Lv_{k,t_n}(t) &= e^{(k-t)L}Lu(t_n + t), \end{aligned}$$

from what (12) is directly proved for $q = 1$ and (13) comes using also (1). Then, inductively, for $0 \leq r \leq q$, $0 \leq j \leq r$,

$$\begin{aligned} v_{k,t_n}^{(j)}(t) &= \sum_{l=0}^{j} \binom{j}{l} (-1)^l e^{(k-t)L} L^l u^{(j-l)}(t_n + t), \qquad (14) \\ L^{r-j}v_{k,t_n}^{(j)}(t) &= \sum_{l=0}^{j} \binom{j}{l} (-1)^l e^{(k-t)L} L^{r-j+l} u^{(j-l)}(t_n + t), \end{aligned}$$

which proves (12). □

Theorem 3.2 *Whenever the quadrature rule is exact for polynomials of degree $\leq p-1$ and the solution u of (1) satisfies (7) for some $q \leq p+1$, the local truncation error satisfies $\delta_{n,k} = O(k^q)$, where the constant in Landau notation depends on the coefficients of the method and uniform bounds of the functions in (7).*

Proof. Notice that (10) can be written in terms of v_{k,t_n} in (11) as

$$\begin{aligned}\delta_{n,k} &= v_{k,t_n}(k) - v_{k,t_n}(0) - k\sum_{i=1}^{s} b_i v'_{k,t_n}(c_i k)\\ &= \int_0^k v'_{k,t_n}(s)ds - k\sum_{i=1}^{s} b_i v'_{k,t_n}(c_i k). \end{aligned} \tag{15}$$

Now, for $q = 1$, assumption (7) implies that f is uniformly bounded for $t \in [0, T]$. On the other hand, because of (13), $v'_{k,t_n}(t)$ will also be bounded in the same way. From this, it is clear that $\delta_{n,k} = O(k)$.

On the other hand, for $q \geq 2$, notice that $0 \leq q-2 \leq p-1$, and therefore the following Peano kernel expression [**?**] can be used to represent the error in the quadrature formula which was written in (15):

$$\delta_{n,k} = \int_0^k v^{(q)}_{k,t_n}(s) K_{q-2,k}(s) ds, \tag{16}$$

where

$$K_{q-2,k}(s) = \frac{1}{(q-2)!}[\int_u^k (x-s)^{q-2}dx - k\sum_{i=1}^{s} b_i (c_i k - s)_+^{q-2}] = O(k^{q-1}). \tag{17}$$

Inserting this in (16) and considering also the uniform bound for $\|v^{(q)}_{k,t_n}\|$ due to (12), the result follows.
□

In the following, we will justify the fractional order which is many times observed.

Lemma 3.3 *Let us assume that the quadrature rule is exact for polynomials of degree $\leq p-1$, the solution u of (1) belongs to $C^{q+1}([0, T], X)$ for some $q \leq p$ and satisfies*

$$L^{r-j}(-L)^{\alpha} u^{(j)} \in C([0, T], X), \quad 0 \leq j \leq r, \quad 0 \leq r \leq q, \tag{18}$$

for some $\alpha \in [0,1)$. Then, the local truncation error satisfies $L^{-1}(-L)^\alpha \delta_{n,k} = O(k^{q+1})$, where the constant in Landau notation depends on the coefficients of the method and uniform bounds of $u^{(q+1)}$ and the functions in (18).

Proof. From (15),

$$L^{-1}(-L)^\alpha \delta_{n,k} = \int_0^k L^{-1}(-L)^\alpha v'_{k,t_n}(s)ds - k\sum_{i=1}^s b_i L^{-1}(-L)^\alpha v'_{k,t_n}(c_i k).$$

Now, let us see that $L^{-1}(-L)^\alpha v'_{k,t_n}$ belongs to $C^q([0,T],X)$. For that, from expression (14) for $j=q$, we have that

$$L^{-1}(-L)^\alpha v^{(q)}_{k,t_n}(t) = \sum_{l=0}^q \begin{pmatrix} q \\ l \end{pmatrix} (-1)^l e^{(k-t)L} L^{l-1}(-L)^\alpha u^{(q-l)}(t_n+t),$$

which is clearly differentiable again with respect to t and

$$L^{-1}(-L)^\alpha v^{(q+1)}_{k,t_n}(t) = \sum_{l=0}^q \begin{pmatrix} q \\ l \end{pmatrix} (-1)^l [-e^{(k-t)L} L^{l}(-L)^\alpha u^{(q-l)}(t_n+t) + e^{(k-t)L} L^{l-1}(-L)^\alpha u^{(q-l+1)}(t_n+t)]. \quad (19)$$

The previous function is continuous due to (18) and the fact that $u \in C^{q+1}([0,T],X)$. (Notice that $L^{-1}(-L)^\alpha = -(-L)^{\alpha-1}$ is a bounded operator.) Therefore, Peano kernel Theorem can now be used with $K_{q-1,k}$ instead of just $K_{q-2,k}$, i.e.

$$L^{-1}(-L)^\alpha \delta_{n,k} = \int_0^k L^{-1}(-L)^\alpha v^{(q+1)}_{k,t_n}(s) K_{q-1,k}(s)ds. \quad (20)$$

As $K_{q-1,k}(s) = O(k^q)$ because of (17) and $L^{-1}(-L)^\alpha v^{(q+1)}_{k,t_n}$ is bounded, the result follows. □

Theorem 3.4 *Under the hypotheses of Lemma 3.3 for $\alpha \in (0,1)$ and assuming also that for that α there exists $k_0 > 0$ and $C > 0$ such that*

$$\|(-sL)^{1-\alpha} e^{sL}\| \le C, \quad s \in [0,k_0), \quad (21)$$

it happens that $\delta_{n,k} = O(k^{q+\alpha})$, where the constant in Landau notation depends on the coefficients of the method, uniform bounds of $u^{(q+1)}$ and the functions in (18), the constant C in (21) and $1/\alpha$.

Proof. By considering (20) multiplied by $L(-L)^{-\alpha}$ and inserting expression (19), it is deduced that

$$\delta_{n,k} = \int_0^k (k-s)^{\alpha-1} \Big[\sum_{l=0}^{q} \begin{pmatrix} q \\ l \end{pmatrix} (-1)^l [-(k-s)^{1-\alpha} L(-L)^{-\alpha} e^{(k-s)L} L^l (-L)^\alpha u^{(q-l)}(t_n+s) \\ +(k-s)^{1-\alpha} L(-L)^{-\alpha} e^{(k-s)L} L^{l-1} (-L)^\alpha u^{(q-l+1)}(t_n+s)] \Big] K_{q-1,k}(s) ds. \quad (22)$$

By using (21) and (18), the term in big brackets is again bounded and, as $K_{q-1,k}(s) = O(k^q)$, it happens that

$$\delta_{n,k} = O(k^q) \int_0^k (k-s)^{\alpha-1} ds = O(k^{q+\alpha}),$$

where it has been used that the previous integral is k^α/α. □

Remark 3.5 *In a similar way to Theorem 2.4, the conditions of regularity (18) are satisfied when $u_0 \in D((-L)^{q+\alpha})$, $f \in C^q([0,T], X)$ and for $1 \le j \le q-1$ and $0 \le m \le j-1$, $f^{(j-1-m)}(t) \in D((-L)^{\alpha+m+1})$ for each $t \in [0,T]$ and*

$$L^{m+1}(-L)^\alpha f^{(j-1-m)} \in C^1([0,T], X).$$

3.2 Global error

In this subsection, we analyse the global error, i.e. the difference between the exact and the numerical solution at each step. For this problem and Lawson method, we have the recursion formula:

$$\begin{aligned} e_{n+1,k} &= u(t_{n+1}) - u_{n+1} \\ &= u(t_{n+1}) - (e^{kL} u_n + k \sum_{i=1}^{s} b_i e^{(1-c_i)kL} f(t_n + c_i k)) \\ &= u(t_{n+1}) - (e^{kL} u(t_n) + k \sum_{i=1}^{s} b_i e^{(1-c_i)kL} f(t_n + c_i k)) + e^{kL}(u(t_n) - u_n) \\ &= \delta_{n,k} + e^{kL} e_{n,k}. \end{aligned} \quad (23)$$

From this, the following theorem easily follows.

Theorem 3.6 *Whenever the quadrature rule is exact for polynomials of degree $\le p-1$ and the solution u of (1) satisfies (7) for some $q \le p+1$, the global error satisfies $e_n = O(k^{q-1})$, where the constant in Landau notation depends on the coefficients of the method and uniform bounds of the functions in (7).*

Proof. From recursion (23), it is clear that

$$e_{n+1,k} = \sum_{j=0}^{n} e^{(n-j)kL}\delta_{j,k}. \tag{24}$$

From (2), $\|e^{tL}\|$ is uniformly bounded when $t \in [0,T]$. Considering also Theorem 3.2 and the fact that $0 \le (n-j)k \le T$, the result follows. □

With the same argument, but using Theorem 3.4, the following theorem also follows under more assumptions of regularity.

Theorem 3.7 *Under the hypotheses of Theorem 3.4, the global error satisfies* $e_n = O(k^{q+\alpha-1})$, *where the constant in Landau notation depends on the coefficients of the method, uniform bounds of* $u^{(q+1)}$ *and the functions in (18), the constant* C *in (21) and* $1/\alpha$.

However, in practice, many times the global error converges more quickly. The following results explain that.

Theorem 3.8 *We assume that, for* $n \ge 1$, *the bound*

$$\|kL\sum_{l=1}^{n} e^{lkL}\| \le C, \tag{25}$$

holds for a constant C *independent of* k *and* n *satisfying* $0 \le nk \le T$.

Whenever the quadrature rule is exact for polynomials of degree $\le p-1$ *and the solution* u *of (1) belongs to* $C^{q+2}([0,T],X)$ *for some* $q \le p$, *satisfies (7) for that* q *and, for* $l = 0,\dots,q$,

$$L^l u^{(q+1-l)}, L^{l-1}u^{(q+2-l)} \in C([0,T],X), \tag{26}$$

the global error satisfies $e_n = O(k^q)$, *where the constant in Landau notation depends on the coefficients of the method and uniform bounds of the functions in (7) and (26).*

Proof. The result follows from rewriting (24) as

$$\begin{aligned} e_{n+1,k} &= (\sum_{l=0}^{n} e^{lkL})\delta_{0,k} + \sum_{j=0}^{n-1}(\sum_{l=0}^{j} e^{lkL})(\delta_{n-j,k} - \delta_{n-j-1,k}) \\ &= \delta_{0,k} + (kL\sum_{l=1}^{n} e^{lkL})k^{-1}L^{-1}\delta_{0,k} + \sum_{j=0}^{n-1}(\delta_{n-j,k} - \delta_{n-j-1,k}) \end{aligned} \tag{27}$$

$$+\sum_{j=0}^{n-1}(kL\sum_{l=1}^{j}e^{lkL})k^{-1}L^{-1}(\delta_{n-j,k}-\delta_{n-j-1,k}). \qquad (28)$$

Considering then Theorem 3.2, Lemma 3.3 with $\alpha = 0$ and (25), the first two terms in (27) are clearly $O(k^q)$. Now, using (16), (14) with $j = q$, and that $K_{q-2,k} = O(k^{q-1})$, the third term in (27) is also $O(k^q)$. Finally, in order to bound (28) in the same way, it suffices to consider (20) and (19) with $\alpha = 0$, and the assumptions on u. Therefore,

$$L^{-1}[v^{(q+1)}_{k,t_{n-j}}(s)-v^{(q+1)}_{k,t_{n-j-1}}(s)]$$
$$=k\sum_{l=0}^{q}\binom{q}{l}(-1)^l[-e^{(k-s)L}L^lu^{(q-l+1)}(t^*_{n-j}+s)+e^{(k-s)L}L^{l-1}u^{(q-l+2)}(t^*_{n-j}+s)],$$

for some $t^*_{n-j}\in(t_{n-j-1},t_{n-j})$. As the previous term is $O(k)$,

$$L^{-1}(\delta_{n-j,k}-\delta_{n-j-1,k})=O(k^{q+2}),$$

which implies the result. □

Now, the following lemma, similar to Lemma 3.3, allows to prove fractional order of convergence together with summation-by-parts when $q \le p-1$.

Lemma 3.9 *Let us assume that the quadrature rule is exact for polynomials of degree $\le p-1$ and the solution u of (1) belongs to $C^{q+2}([0,T],X)$ for some $q \le p-1$ and satisfies (18) for some $\alpha \in [0,1)$. Then, the local truncation error satisfies $L^{-2}(-L)^{\alpha}\delta_{n,k} = O(k^{q+2})$, where the constant in Landau notation depends on the coefficients of the method and uniform bounds of $u^{(q+1)}$, $u^{(q+2)}$ and the functions in (18).*

Proof. In a similar way to the proof of Lemma 3.3, we have to bound

$$L^{-2}(-L)^{\alpha}\delta_{n,k}=\int_0^k L^{-2}(-L)^{\alpha}v'_{k,t_n}(s)ds-k\sum_{i=1}^{s}b_iL^{-2}(-L)^{\alpha}v'_{k,t_n}(c_ik).$$

The difference is that now we can consider as Peano kernel $K_{q,k}(s)$, since $q \le p-1$, whenever $L^{-2}(-L)^{\alpha}v'_{k,t_n}$ belongs to $C^{q+1}([0,T],X)$. Writing L^{-1} before (19) and differentiating with respect to t,

$$L^{-2}(-L)^{\alpha}v^{(q+2)}_{k,t_n}(t)=\sum_{l=0}^{q}\binom{q}{l}(-1)^l[e^{(k-t)L}L^l(-L)^{\alpha}u^{(q-l)}(t_n+t)$$
$$-2e^{(k-t)L}L^{l-1}(-L)^{\alpha}u^{(q-l+1)}(t_n+t)+e^{(k-t)L}L^{l-2}(-L)^{\alpha}u^{(q-l+2)}(t_n+t)], \qquad (29)$$

which is continuous due to (18) and the fact that $u \in C^{q+2}([0,T],X)$. Then, using that $K_{q,k}(s) = O(k^{q+1})$, the result follows. □

Theorem 3.10 *Let us assume that, for $n \ge 1$, bound (25) holds, (21) is satisfied for some $\alpha \in (0,1)$, the quadrature rule is exact for polynomials of degree $\le p-1$ and the solution u of (1) belongs to $C^{q+3}([0,T],X)$ for some $q \le p-1$, satisfies (18) for that q and the above value of α, and for $l = 0,\dots,q$,*

$$L^l(-L)^\alpha u^{(q-l+1)}, L^{l-1}(-L)^\alpha u^{(q-l+2)}, L^{l-2}(-L)^\alpha u^{(q-l+3)} \in C([0,T],X). \quad (30)$$

Then, the global error satisfies $e_n = O(k^{q+\alpha})$, where the constant in Landau notation depends on the coefficients of the method, uniform bounds of the functions in (18) and (30) and on $1/\alpha$.

Proof. The result follows from rewriting (24) as (27)-(28) again, like in the proof of Theorem 3.8.

Now, the first term in (27) is $O(k^{q+\alpha})$ by applying Theorem 3.4.

The second term in (27) is also $O(k^{q+\alpha})$ due to (25) and because, by using (15) and (29),

$$\begin{aligned}
L^{-1}\delta_{0,k} &= \int_0^k L(-L)^{-\alpha}L^{-2}(-L)^\alpha v^{(q+2)}_{k,t_{n-j}}(s)K_{q,k}(s)ds \\
&= \int_0^k (k-s)^{\alpha-1}\sum_{l=0}^q \begin{pmatrix} q \\ l \end{pmatrix} (-1)^l \Big[(k-s)^{1-\alpha}L(-L)^{-\alpha}e^{(k-s)L}L^l(-L)^\alpha u^{(q-l)}(t_n+s) \\
&\quad -2(k-s)^{1-\alpha}L(-L)^{-\alpha}e^{(k-s)L}L^{l-1}(-L)^\alpha u^{(q-l+1)}(t_n+s) \\
&\quad +(k-s)^{1-\alpha}L(-L)^{-\alpha}e^{(k-s)L}L^{l-2}(-L)^\alpha u^{(q-l+2)}(t_n+s)\Big] K_{q,k}(s)ds,
\end{aligned}$$

which is $O(k^{q+1+\alpha})$ considering (21), (30) and that $K_{q,k}(s) = O(k^{q+1})$.

As for the third term in (27), it is also $O(k^{q+\alpha})$ by using (22) and (21).

Finally, in order to bound (28) in the same way, it suffices to consider that

$$\begin{aligned}
&L^{-1}(\delta_{n-j,k} - \delta_{n-j-1,k}) \\
&= \int_0^k L^{-1}[v^{(q+2)}_{k,t_{n-j}}(s) - v^{(q+2)}_{k,t_{n-j-1}}(s)]K_{q,k}(s)ds \\
&= \int_0^k (k-s)^{1-\alpha}L(-L)^{-\alpha}(k-s)^{\alpha-1}L^{-2}(-L)^\alpha[v^{(q+2)}_{k,t_{n-j}}(s) - v^{(q+2)}_{k,t_{n-j-1}}(s)]K_{q,k}(s)ds
\end{aligned}$$

$$= O(k^{q+2+\alpha}) \tag{31}$$

because of (29), (30) and (21), from what the result follows using also (25). □

Remark 3.11 *The bound (25) has been proved in [?] for analytic semigroups, covering the case in which (1) corresponds to parabolic problems. Bound (21) can also be seen to be valid for parabolic problems. Moreover, the trick of the summation by parts may be used in other cases. For example, it is used in [?] when integrating regular solutions of Schrödinger equation. The fractional order of convergence and summation by parts appear in the case of C_0-semigroups and Runge-Kutta type methods [?, ?, ?, ?, ?].*

In any case, we notice that, in practice, the time integration is made when (1) has been previously discretized in space and the summation by parts may be valid for the semidiscrete problem.

4 Examples and numerical results

In this section, we will corroborate the results of the previous section in the numerical integration of the evolutionary initial boundary value problem with homogeneous boundary conditions:

$$\begin{aligned} u_t(x,t) &= \Delta u(x,t) + f(x,t), \quad x \in \Omega, \quad t \in [0,T], \\ u(x,0) &= u_0(x), \\ u(x,t) &= 0, \quad x \in \partial\Omega, \end{aligned} \tag{32}$$

where Ω is a certain convex set of $\mathbb{R}^d$ with a Liptschitz continuous boundary $\partial\Omega$, Δ is the Laplacian operator, $u_0 \in L^2(\Omega)$ and for each $t \in [0,T]$, $f(\cdot,t) \in L^2(\Omega)$. In such a way, this problem can be written under the framework of (1) where $X = L^2(\Omega)$ and $L : H^2(\Omega) \cap H_0^1(\Omega) \to L^2(\Omega)$ is the Laplacian operator restricted to functions of $H^2(\Omega)$ which vanish on $\partial\Omega$. Moreover, when $\alpha \in [0, \frac{1}{4})$, $D((-L)^\alpha) = H^{2\alpha}(\Omega)$ while for $\alpha \in (\frac{1}{4}, 1)$, $D((-L)^\alpha) = H^{2\alpha}(\Omega) \cap H_0^\alpha(\Omega)$ [?,?].

We have first considered the one-dimensional problem corresponding to $\Omega = [0,1]$ and three different choices of u_0 and f,

(i) $u_0(x) = x(1-x)e^x, \quad f(x,t) = 2x(1+x)e^{x-t}$,
(ii) $u_0(x) = x^3(1-x)^3, \quad f(x,t) = e^t x(6 - 36x + 59x^2 - 27x^3 - 3x^4 + x^5)$,
(iii) $u_0(x) = \sin(\pi x), \quad f(x,t) = e^t(1+\pi^2)\sin(\pi x)$.

It is simple to check that in case (i) Theorem 2.4 can be applied with $q = 1$. In case (ii), with $q = 2$ and, in case (iii) with any natural value of q. Therefore,

(7) is satisfied with the respective values of q. This can be corroborated here since the exact solutions are given by

(i) $u(x,t) = x(1-x)e^{x-t}$,
(ii) $u(x,t) = x^3(1-x)^3 e^t$,
(iii) $u(x,t) = \sin(\pi x)e^t$.

Besides, notice that, for $0 \le \alpha < \frac{1}{4}$, $u(t) \in D(L^{1+\alpha})$ in case (i), $u(t) \in D(L^{2+\alpha})$ in case (ii) and $u(t) \in D(L^q)$ for any $q \ge 1$ in case (iii).

We have numerically integrated these problems till $T = 1$ with the standard second-order finite difference method in space and the explicit Lawson method which is based on the Runge-Kutta method

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \qquad (33)$$

Notice that the quadrature rule associated to this method is just the trapezoidal rule. It is well known that this method has order $p = 2$. Besides, we have considered a small enough value of the space stepsize such that the error in space can be considered negligible against the errors coming from the time integration. More precisely, we have taken $h = 2.5 \times 10^{-3}$.

k	2.5×10^{-2}	1.25×10^{-2}	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}
Local error	2.59×10^{-2}	1.10×10^{-2}	4.65×10^{-3}	1.94×10^{-3}	8.01×10^{-4}
Order		1.23	1.25	1.26	1.27

Table 1
Local error corresponding to the integration of problem (i) with Lawson trapezoidal rule in time

k	2.5×10^{-2}	1.25×10^{-2}	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}
Local error	1.15×10^{-4}	2.61×10^{-5}	5.75×10^{-6}	1.24×10^{-6}	2.64×10^{-7}
Order		2.14	2.19	2.21	2.23

Table 2
Local error after applying L^{-1} corresponding to the integration of problem (i) with Lawson trapezoidal rule in time

Notice that, in case (i), (7) is satisfied just for $q = 1$ since u vanishes on the boundary and is regular enough but it is not satisfied for $q = 2$ since Lu does not vanish on the boundary any more and therefore it has no sense to consider L^2u. Because of this, Theorem 3.2 can be applied with $q = 1$ and it is therefore

k	2.5×10^{-2}	1.25×10^{-2}	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}
Global error	9.95×10^{-3}	4.20×10^{-3}	1.76×10^{-3}	7.32×10^{-4}	3.03×10^{-4}
Order		1.25	1.26	1.26	1.27

Table 3
Global error corresponding to the integration of problem (i) with Lawson trapezoidal rule in time

k	2.5×10^{-2}	1.25×10^{-2}	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}
Local error	1.00×10^{-3}	2.40×10^{-4}	5.36×10^{-5}	1.16×10^{-5}	2.49×10^{-6}
Order		2.06	2.16	2.21	2.23

Table 4
Local error corresponding to the integration of problem (ii) with Lawson trapezoidal rule in time

k	2.5×10^{-2}	1.25×10^{-2}	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}
Global error	2.90×10^{-3}	8.27×10^{-4}	2.24×10^{-4}	5.93×10^{-5}	1.55×10^{-5}
Order		1.81	1.88	1.92	1.93

Table 5
Global error corresponding to the integration of problem (ii) with Lawson trapezoidal rule in time

k	6.25×10^{-2}	3.125×10^{-2}	1.5625×10^{-2}	7.8125×10^{-3}	3.9062×10^{-3}
Local error	1.42×10^{-2}	2.02×10^{-3}	2.70×10^{-4}	3.51×10^{-5}	4.57×10^{-6}
Order		2.81	2.90	2.94	2.94

Table 6
Local error corresponding to the integration of problem (iii) with Lawson trapezoidal rule in time

k	6.25×10^{-2}	3.125×10^{-2}	1.5625×10^{-2}	7.8125×10^{-3}	3.9062×10^{-3}
Global error	2.90×10^{-3}	8.27×10^{-4}	2.24×10^{-4}	5.93×10^{-5}	1.55×10^{-5}
Order		1.99	2.00	1.99	1.97

Table 7
Global error corresponding to the integration of problem (iii) with Lawson trapezoidal rule in time

proved that the local error $\delta_{n,k}$ is $O(k)$. What's more, as $u \in D((-L)^{1+\alpha})$ for any $\alpha < \frac{1}{4}$, Theorem 3.4 can be applied with all those values of α and $q = 1$ and therefore the local error is $O(k^{1+\alpha})$. That can be corroborated in Table 1 where the errors after one step of integration and measured in the discrete L^2-norm are stated for several values of time stepsize k. The numerical order is seen to be very close to 1.25. Besides, as $u \in C^2([0,1], X)$, Lemma 3.3 can also be applied with $q = 1$ and $\alpha < \frac{1}{4}$. In fact, for $\alpha = 0$ we get $L^{-1}\delta_n = O(k^2)$.

k	5.00×10^{-2}	2.50×10^{-2}	1.25×10^{-2}	6.25×10^{-3}
Local error	7.54×10^{-5}	3.03×10^{-6}	1.07×10^{-7}	3.43×10^{-9}
Order		4.64	4.82	4.97

Table 8
Local error corresponding to the integration of problem (iv) with Lawson Simpson's rule in time

k	5×10^{-2}	2.5×10^{-2}	1.25×10^{-2}	6.25×10^{-3}
Global error	4.80×10^{-5}	3.06×10^{-6}	1.91×10^{-7}	1.15×10^{-8}
Order		3.97	4.00	4.06

Table 9
Global error corresponding to the integration of problem (iv) with Lawson Simpson's rule in time

This fits perfectly with what is observed in Table 2 where the results in the first row correspond to the discrete L^2-norm of the inverse of the matrix which has been used for the space discretization of the second-derivative applied over the local error after one step. Moreover, as u also belongs to $C^4([0,1], X)$ and satisfies (30) with $q = 1$, Theorem 3.10 can be applied with the same value of q and $\alpha < \frac{1}{4}$, which explains that the global error behaves as $O(k^{1.25})$. This can now be corroborated in Table 3.

On the other hand, in case (ii), (7) is satisfied just for $q = 2$ since u and Lu vanish on the boundary and are regular enough but it is not satisfied for $q = 3$ since L^2u does not vanish on the boundary. Therefore, Theorem 3.2 can be applied with $q = 2$ and the local error is $\delta_{n,k} = O(k^2)$. Moreover, as $u \in D(L^{2+\alpha})$ for any $\alpha < \frac{1}{4}$, Theorem 3.4 can also be applied with those values of α. That is corroborated in Table 4 where the numerical order is seen to be very near 2.25. Moreover, as u also belongs to $C^4([0,1], X)$ and satisfies (26) with $q = 2$, Theorem 3.8 can be applied with the same value of q, which explains that the global error behaves as $O(k^2)$. This can now be corroborated in Table 5.

As for case (iii), (7) is satisfied for arbitrarily large q. Therefore, Theorem 3.2 can be applied with the maximum value of q, which is $q = 3$ because $p = 2$, and order 3 for the local error is obtained, as Table 6 shows. Besides, as again u is very regular and satisfies (26) for arbitrarily large q, Theorem 3.8 can also be applied with the biggest value of q which is now allowed, which is $q = 2$, and order 2 for the global error is obtained. This is also corroborated in Table 7. Notice that this order is the same that Theorem 3.6 provides without assuming so much regularity but using $q = 3$ in (7). Notice also that Theorem 3.10 can only be applied in this case with $q = 1$ and that the estimate for the global error which is given in that theorem is worse than the one which is given by Theorems 3.6 and 3.8.

Finally, in order to corroborate that the results are also true in higher dimensional problems and when the numerical integrator is more accurate, we have integrated problem (32) in the square $\Omega = [0,1] \times [0,1]$. We have considered as space discretization the well-known nine-point formula [**?**] and, as time integrator, the explicit Lawson method which is based, for example, on the classical 4th-order Runge-Kutta method and which is associated to Simpson's quadrature rule for our linear problem. As initial condition and source term, we have considered now

(iv) $\quad u_0(x,y) = \sin(\pi x)\sin(\pi y), \;\; f(t,x,y) = (-1+2\pi^2)\sin(\pi x)\sin(\pi y)e^{-t},$

whose exact solution is

(iv) $\quad u(t,x,y) = \sin(\pi x)\sin(\pi y)e^{-t}.$

In this case, as the solution is very regular and the succesive Laplacians of it continue vanishing on the boundary, Theorem 3.2 can be applied with the maximum value of q, which is now $q = 5$ because Simpson's quadrature rule is exact for polynomials of degree ≤ 3 and therefore $p = 4$. In such a way, the local error is $O(k^5)$, as is observed in Table 8. As for the global error, Theorem 3.6 can now be applied with $q = 5$ and therefore order 4 is obtained, as Table 9 shows. Again the space grid has been chosen fine enough so that the error in space is negligible against time integration errors. More precisely, a uniform grid with $h = 10^{-2}$ has been considered.