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M. P. Calvo · C. Palencia

A class of explicit multistep exponential integrators for semilinear problems

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Abstract A class of explicit multistep exponential methods for abstract semilinear equations is introduced and analyzed. It is shown that the k-step method achieves order k, for appropriate starting values, which can be computed by auxiliary routines or by one strategy proposed in the paper. Together with some implementation issues, numerical illustrations are also provided.

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1 Introduction

In the present paper we derive and analyze a family of explicit multistep exponential methods for the time integration of abstract semilinear problems

$$u'(t) = Au(t) + f(t, u(t)), \quad u(0) = u_0, \quad 0 \le t \le T. \tag{1}$$

Problem (1) is assumed to fit in Henry's setting [6], which covers many interesting applications. To be more precise, we assume that $A : D(A) \subset X \to X$ is the infinitesimal generator of a C_0-semigroup e^{tA}, $t \ge 0$, of linear and bounded operators in a complex Banach space X, with growth governed by

$$\|\mathrm{e}^{tA}\| \le M\mathrm{e}^{\omega t}, \quad t \ge 0, \tag{2}$$

for some $M > 0, \omega \in \mathbf{R}$. The class of nonlinearities allowed in this setting depends on the nature of the semigroup e^{tA}, $t \ge 0$. If e^{tA}, $t \ge 0$, is just a C_0-semigroup, we assume, by simplicity, that $f : [0, T] \times X \to X$ is globally Lipschitz, i.e.

$$\|f(t, \eta) - f(t, \xi)\| \le L\|\eta - \xi\|, \quad \eta, \xi \in X, \quad 0 \le t \le T,$$

M. P. Calvo (✉) · C. Palencia
Departamento de Matemática Aplicada, Universidad de Valladolid, Spain
E-mail: maripaz@mac.cie.uva.es

for some $L > 0$. However, if the semigroup is analytic, we can afford for stronger nonlinearities. In this case, for $0 \leq \alpha < 1$, let X_α be the domain of the α-th fractional power of $(\nu - A)$, i.e. $X_\alpha = D((\nu - A)^\alpha)$, for some fixed $\nu > \omega$, endowed with the graph norm $\| \cdot \|_\alpha$ of $(\nu - A)^\alpha$ (different choices of $\nu > \omega$ result in the same space X_α and equivalent norms $\| \cdot \|_\alpha$). Then, for an analytic semigroup, the nonlinearity f is assumed to be defined on $[0, T] \times X_\alpha \to X$, for some $0 \leq \alpha < 1$, and to be globally Lipschitz

$$\|f(t, \eta) - f(t, \xi)\| \leq L\|\eta - \xi\|_\alpha, \quad \eta, \xi \in X_\alpha, \quad 0 \leq t \leq T, \tag{3}$$

for some $L > 0$.

In summary, f is always assumed to satisfy (3) for some appropriate $0 \leq \alpha < 1$ depending on the nature of the semigroup. Although, by simplicity, we assume that f is globally Lipschitz in the sense of (3), the proof of our main result (Theorem 1) can easily be adapted to cover the case where f satisfies (3) only in some strip along the exact solution.

It is well known that, under (2) and (3), problem (1) possesses a unique mild solution $u : [0, T] \to X_\alpha$ for $u_0 \in X_\alpha$ [6,24].

In this setting, time discretizations of (1), by means of either Runge-Kutta type or linear multistep methods, have been widely considered in the literature [5,17–19, 23].

On the other hand, exponential integrators and related variants [4,16,21,22, 27–29] were proposed a time ago as an alternative to those classical methods. However, exponential integrators were considered of limited practical interest since they require evaluations of the form

$$\gamma(hA)v, \quad v \in X, \tag{4}$$

where either $\gamma(hA) = \mathrm{e}^{lhA}$ or

$$\gamma(hA) = \int_0^l \mathrm{e}^{(l-\sigma)hA} p(\sigma)\, \mathrm{d}\sigma, \tag{5}$$

with $p(\sigma)$ a polynomial and $l \geq 1$ an integer (these integrals can be understood in Bochner's sense and they define bounded operators in X [7]). Thus, to implement an exponential integrator we need to assume that evaluations in (4) can be carried out, within some prescribed accuracy, by means of suitable auxiliary routines. Of course, this is a strong assumption from the computational point of view. However, noticing that the underlying entire functions

$$\gamma(\lambda) = \int_0^l \mathrm{e}^{(l-\sigma)\lambda} p(\sigma)\, \mathrm{d}\sigma,$$

behave like e^λ, we can efficiently evaluate (4), by using a Krylov approach [8, 9], at least in case A is a sparse matrix. Moreover, for model problems involving differential operators with constant coefficients, in canonical domains, this goal can be achieved by using discrete Fourier techniques (see Section 6).

Actually, as soon as the required evaluations (4) are considered a feasible task, at least in the context of some relevant applications, exponential integrators have got a renewed interest [1,2,10–15,21]. While most of these references deal with exponential Runge-Kutta methods, in the present paper we consider a class of explicit

k-step exponential integrators, similar to those in [1,2,22], applied to abstract semilinear problems (1). We prove that the k-step method, for arbitrary $k \geq 1$, exhibits full order k under the only assumption that the composition $f(t, u(t))$ in (1) is smooth enough in time, so that no order reduction takes place cf. [13]. These methods might be very competitive, since no solvers are used whatsoever. However, in the present paper we do not address the comparison of the efficiency of exponential integrators against the one of classical methods.

The paper is organized as follows. In Section 2 we derive the family of k-step schemes, whose convergence is analyzed in Section 3. It turns out that, to achieve the full order, suitable starting values are required. This issue is studied in Section 4. Section 5 is devoted to implementation details concerning the evaluations in (4). Finally, some numerical illustrations are shown in Section 6.

2 Construction of the methods

We start by constructing a class of explicit multistep exponential integrators for (1) in the spirit of [1,2,22].

Let $u : [0, T] \to X_\alpha$ be the solution of (1). In order to derive the k-step method, let us consider a step-size $h = T/N$, $N \geq k$, and the corresponding time levels $t_n = nh$, $0 \leq n \leq N$. The variation-of-constants formula for the interval $[t_n, t_{n+k}]$, $n + k \leq N$, reads

$$\begin{aligned} u(t_{n+k}) &= \mathrm{e}^{(t_{n+k}-t_n)A}u(t_n) + \int_{t_n}^{t_{n+k}} \mathrm{e}^{(t_{n+k}-s)A} f(s, u(s))\,\mathrm{d}s \\ &= \mathrm{e}^{khA}u(t_n) + h\int_0^k \mathrm{e}^{(k-\sigma)hA} f(t_n + \sigma h, u(t_n + \sigma h))\,\mathrm{d}\sigma. \end{aligned} \tag{6}$$

Then, given approximations $u_{n+j} \sim u(t_{n+j})$, $0 \leq j \leq k-1$, it is natural to define the new approximation $u_{n+k} \sim u(t_{n+k})$ by

$$u_{n+k} = \mathrm{e}^{khA}u_n + h\int_0^k \mathrm{e}^{(k-\sigma)hA} P_{n,k-1}(t_n + \sigma h)\,\mathrm{d}\sigma, \tag{7}$$

where $P_{n,k-1}$ stands for the Lagrange interpolation polynomial of degree $k-1$ through the points $\{(t_{n+j}, f(t_{n+j}, u_{n+j}))\}_{j=0}^{k-1}$. It is clear, under the proviso that both $\mathrm{e}^{khA}v$ and

$$\int_0^k \mathrm{e}^{(k-\sigma)hA}\sigma^j v\,\mathrm{d}\sigma, \quad 0 \leq j \leq k-1,$$

are computable for any $v \in X$, that (7) defines an explicit time integrator for (1). Naturally, starting values $u_0, \ldots, u_{k-1}$ should be provided (see Section 4).

Notice that in (7) the variation-of-constants formula is used from t_n to t_{n+k}, while in the ETD integrators of Adams type [1,2,22] it is used from t_{n+k-1} to t_{n+k}.

Both, for the practical implementation and for the analysis, it is convenient to write

$$P_{n,k-1}(t_n + \sigma h) = \sum_{j=0}^{k-1} \binom{\sigma}{j} \Delta^j f_n,$$

where $f_m = f(t_m, u_m)$, $0 \le m \le N-1$, and Δ denotes the standard forward difference operator. Thus, (7) becomes

$$u_{n+k} = \mathrm{e}^{khA} u_n + h \sum_{j=0}^{k-1} \gamma_j(k, hA) \Delta^j f_n, \tag{8}$$

where

$$\gamma_j(k, \lambda) = \int_0^k \mathrm{e}^{(k-\sigma)\lambda} \binom{\sigma}{j} \, \mathrm{d}\sigma, \quad 0 \le j \le k-1.$$

In Section 3 it is proved that for given starting values $u_0, \dots, u_{k-1} \in X_\alpha$ there holds $u_{n+k} \in X_\alpha$ for $n \ge 0$, so that (8) is well defined.

3 Convergence analysis

Before stating the main theorem of this paper, we need to introduce some notation and preliminary results.

The product spaces X_β^k, $0 \le \beta \le \alpha$, are endowed with the norm

$$\|V\|_\beta = \max_{0 \le j \le k-1} \|v_j\|_\beta, \quad V = [v_0, \dots, v_{k-1}]^T \in X_\beta^k.$$

The operator norm of a linear and bounded operator $S : X_{\beta_1}^k \to X_{\beta_2}^k$, $0 \le \beta_j \le \alpha$, $j = 1, 2$, is denoted by $\|S\|_{\beta_1 \to \beta_2}$.

On the other hand, for $\varphi \in C([0, T], X)$, set $\|\varphi\|_\infty = \max_{0 \le t \le T} \|\varphi(t)\|$. Using that for $0 \le \sigma \le k$ and $0 \le \beta \le \alpha$ we know that

$$\|(\sigma h)^\beta \mathrm{e}^{\sigma h A}\|_{0 \to \beta} \le M \mathrm{e}^{\omega^* kh}, \tag{9}$$

where $\omega^* = \max\{\omega, 0\}$, it is clear that for $0 \le \beta \le \alpha$, $j \ge 0$ and $0 < \sigma \le l$, $1 \le l \le k$,

$$\|\mathrm{e}^{(l-\sigma)hA} \sigma^j \varphi(\sigma)\|_\beta \le M \mathrm{e}^{\omega^* kh} \|\varphi\|_\infty \frac{\sigma^j}{(l-\sigma)^\beta h^\beta}.$$

This bound implies that there exists $c_1 = c_1(k, \beta) > 0$ such that

$$\left\| \int_0^l \mathrm{e}^{(l-\sigma)hA} \sigma^j \varphi(\sigma) \, \mathrm{d}\sigma \right\|_\beta \le c_1 M h^{-\beta} \mathrm{e}^{\omega^* kh} \|\varphi\|_\infty, \tag{10}$$

for $1 \le l \le k$, $0 \le j \le k-1$, a basic estimate that will be used repeatedly. Moreover, (10) guarantees that $\gamma_j(k, hA)$ maps X in X_α, since by (10) with φ constant we get

$$\|\gamma_j(l, hA)\|_{0 \to \beta} \le c_2 M h^{-\beta} \mathrm{e}^{\omega^* kh}, \tag{11}$$

for some positive constant $c_2 = c_2(k, \beta)$. Thus $u_n \in X_\alpha$ for $n \ge k$, when the starting points lay in X_α.

Now, given the exact solution $u : [0, T] \to X_\alpha$ of (1), set $g(t) = f(t, u(t))$, $0 \le t \le T$. For $0 \le n \le N - k$, let $\widehat{P}_{n,k-1}(t)$ be the Lagrange interpolation polynomial of degree $k - 1$ with $\widehat{P}_{n,k-1}(t_{n+j}) = g(t_{n+j})$, $0 \le j \le k - 1$. The defects ρ_{n+k} are then defined by

$$u(t_{n+k}) = \mathrm{e}^{khA} u(t_n) + h \int_0^k \mathrm{e}^{(k-\sigma)hA} \widehat{P}_{n,k-1}(t_n + \sigma h)\, \mathrm{d}\sigma + \rho_{n+k}. \qquad (12)$$

Assume that $g \in C^k([0, T], X)$. The elementary bound for the interpolation error reads [25]

$$\|g(t_n + \sigma h) - \widehat{P}_{n,k-1}(t_n + \sigma h)\| \le h^k \|g^{(k)}\|_\infty, \qquad (13)$$

for $0 \le \sigma \le k$. Now, subtracting (12) from (6), we get

$$\rho_{n+k} = h \int_0^k \mathrm{e}^{(k-\sigma)hA} (g(t_n + \sigma h) - \widehat{P}_{n,k-1}(t_n + \sigma h))\, \mathrm{d}\sigma,$$

whence, by (10) and (13), for $0 \le \beta \le \alpha$, there holds

$$\|\rho_{n+k}\|_\beta \le c_1 M \mathrm{e}^{\omega^* kh} h^{k+1-\beta} \|g^{(k)}\|_\infty. \qquad (14)$$

For the subsequent analysis it is convenient to rewrite the k-step method as a one-step scheme. To this end, let us denote $U_n = [u_n, \ldots, u_{n+k-1}]^T$, $U(t_n) = [u(t_n), \ldots, u(t_{n+k-1})]^T$, $R_n = [0, \ldots, 0, \rho_{n+k-1}]^T \in X_\alpha^k$, $E_n = U(t_n) - U_n$ and finally, let $M(hA), B(hA) : X^k \to X^k$ be the operators defined by the operator valued matrices

$$M(hA) = \begin{pmatrix} 0 & I & 0 & \ldots & 0 \\ 0 & 0 & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & I \\ \mathrm{e}^{khA} & 0 & \ldots & 0 & 0 \end{pmatrix}$$

and

$$B(hA) = \begin{pmatrix} 0 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & 0 \\ b_0(hA) & \ldots & b_{k-1}(hA) \end{pmatrix},$$

where

$$b_l(hA) = \sum_{j=l}^{k-1} (-1)^{j-l} \binom{j}{l} \gamma_j(k, hA), \quad 0 \le l \le k - 1. \qquad (15)$$

(Notice that $b_l(hA)$, $0 \le l \le k-1$, depend also on k, but we drop this dependency in the notation).

Throughout this section $C > 0$ stands for a constant depending only on k, α, ω, M and T, perhaps with different values at different places.

Now we establish the bounds for $lh \leq T$

$$\|M(hA)^l\|_{\alpha\to\alpha} \leq C, \quad l \geq 0, \tag{16}$$
$$\|M(hA)^l\|_{0\to\alpha} \leq C \cdot t_l^{-\alpha}, \quad l \geq k, \tag{17}$$
$$\|M(hA)^l B(hA)\|_{0\to\alpha} \leq C \cdot t_{l+1}^{-\alpha}, \quad l \geq 0. \tag{18}$$

To this end, we first notice that, due to the circulant structure of the matrix $M(hA)$, we have

$$M(hA)^{pk+r} = \mathrm{e}^{pkhA} \cdot M(hA)^r, \quad p \geq 0, r \geq 0, \tag{19}$$

which readily proves (16).

To prove (17), for $l \geq k$, we write $l = pk + r$ with $p \geq 1$, $0 \leq r \leq k-1$. From (19), (16) and (9) we deduce

$$\|M(hA)^l\|_{0\to\alpha} \leq \|\mathrm{e}^{pkhA}\|_{0\to\alpha} \cdot \|M(hA)^r\|_{\alpha\to\alpha} \leq \frac{C}{t_{pk}^{\alpha}} \leq \frac{C}{t_l^{\alpha}}.$$

Finally, to prove (18) we distinguish two different cases.

If $l \geq k$, since clearly $\|B(hA)\|_{0\to 0} \leq C$, by (17) we obtain

$$\|M(hA)^l B(hA)\|_{0\to\alpha} \leq \frac{C}{t_l^{\alpha}} \leq \frac{C}{t_{l+1}^{\alpha}}.$$

If $0 \leq l \leq k-1$ we use (11), (15) and (16) to get

$$\|M(hA)^l B(hA)\|_{0\to\alpha} \leq \frac{C}{h^{\alpha}} \leq \frac{C}{t_{l+1}^{\alpha}}.$$

Now we are in a position to state and prove the main result.

Theorem 1 *Let $u : [0,T] \to X_\alpha$ be the solution of (1). Assume that A, f and α satisfy conditions (2) and (3). Assume also that $g(t) = f(t, u(t))$, $0 \leq t \leq T$, belongs to $C^k([0,T], X)$. Let u_n, $0 \leq n \leq N$, be the numerical approximation to $u(t_n)$ obtained using the k-step method (8) with $h = T/N$ and given starting values $u_0, \ldots, u_{k-1} \in X_\alpha$ satisfying*

$$\|u(t_j) - u_j\|_\alpha \leq C_0 \cdot h^k, \quad 0 \leq j \leq k-1. \tag{20}$$

Then, there exists $K > 0$ such that

$$\|u(t_n) - u_n\|_\alpha \leq K \cdot h^k \cdot \|g^{(k)}\|_\infty, \quad 0 \leq n \leq N.$$

The constant K depends only on k, α, L, ω, M, C_0 and T but it is independent of h and g.

Proof For $V = [v_0, \dots, v_{k-1}]^T \in X_\alpha^k$, set

$$F_n(V) = [f(t_n, v_0), \dots, f(t_{n+k-1}, v_{k-1})]^T \in X^k.$$

Using the identity

$$h \sum_{j=0}^{k-1} \gamma_j(k, hA)\Delta^j f_n = h \sum_{l=0}^{k-1} b_l(hA) f_{n+l},$$

it is clear that (8) becomes

$$U_{n+1} = M(hA)U_n + hB(hA)F_n(U_n).$$

Analogously, (12) becomes

$$U(t_{n+1}) = M(hA)U(t_n) + hB(hA)F_n(U(t_n)) + R_{n+1},$$

so that, subtracting the last two expressions we get

$$E_{n+1} = M(hA)E_n + hB(hA)(F_n(U(t_n)) - F_n(U_n)) + R_{n+1},$$

which, by the discrete variation-of-constants formula, results in

$$\begin{aligned} E_n &= M(hA)^n E_0 \\ &\quad + h\sum_{l=0}^{n-1} M(hA)^{n-1-l} B(hA)(F_l(U(t_l)) - F_l(U_l)) \\ &\quad + \sum_{l=1}^{n} M(hA)^{n-l} R_l. \end{aligned}$$

Taking norms in this expression leads to

$$\|E_n\|_\alpha \le (I) + (II) + (III), \tag{21}$$

where

$$\begin{aligned} (I) &= \|M(hA)^n E_0\|_\alpha, \\ (II) &= h\sum_{l=0}^{n-1} \|M(hA)^{n-1-l} B(hA)\|_{0\to\alpha} \cdot \|F_l(U(t_l)) - F_l(U_l)\|_0, \\ (III) &= \sum_{l=1}^{n} \|M(hA)^{n-l} R_l\|_\alpha. \end{aligned}$$

To bound these three terms, we proceed as follows. By (16),

$$(I) \le C\|E_0\|_\alpha.$$

Besides, by (3) and (18),

$$(II) \le CLh \sum_{l=0}^{n-1} \frac{\|E_l\|_\alpha}{t_{n-l}^\alpha}.$$

Finally, by decomposing

$$
\begin{aligned}
(III) &= \sum_{l=1}^{n-k} \|M(hA)^{n-l} R_l\|_\alpha + \sum_{l=0}^{k-1} \|M(hA)^l R_{n-l}\|_\alpha \\
&\le \sum_{l=1}^{n-k} \|M(hA)^{n-l}\|_{0\to\alpha} \cdot \|R_l\|_0 + \sum_{l=0}^{k-1} \|M(hA)^l\|_{\alpha\to\alpha} \cdot \|R_{n-l}\|_\alpha,
\end{aligned}
$$

and recalling (14), (17) and (16), we get

$$
\begin{aligned}
(III) &\le C \sum_{l=1}^{n-k} \frac{1}{t_{n-l}^{\alpha}} \cdot h^{k+1} \cdot \|g^{(k)}\|_\infty + C \sum_{l=0}^{k-1} h^{k+1-\alpha} \cdot \|g^{(k)}\|_\infty \\
&\le C \cdot h^k \cdot \|g^{(k)}\|_\infty.
\end{aligned}
$$

Now, inserting the last estimates in (21), we obtain

$$
\|E_n\|_\alpha \le C\left(\|E_0\|_\alpha + h^k \cdot \|g^{(k)}\|_\infty\right) + CLh \sum_{l=0}^{n-1} \frac{\|E_l\|_\alpha}{t_{n-l}^{\alpha}},
$$

and since $\|E_0\|_\alpha = O(h^k)$ by hypothesis (20), the proof ends after applying the Gronwall's lemma for discrete weakly singular kernels (see e.g. Lemma 4 in [20] and Theorem 6.1 in [3]) and taking into account that $\|u(t_n) - u_n\|_\alpha \le \|E_n\|_\alpha$. □

Notice that with obvious changes in the proof of Theorem 1, we can establish a similar result for ETD methods of multistep type in [1,2,22].

4 Starting values

In Section 3 it has been shown that the proposed k-step method (8) has order k as soon as the starting values $u_0, \ldots, u_{k-1}$ fulfil (20). This is always true for $k = 1$, since $u_0 = u(0)$ is given, but for $k \ge 2$, $k-1$ starting values $u_1, \ldots, u_{k-1}$ satisfying (20) are required. Thus, let us assume that $k \ge 2$. One first possibility is just to use an auxiliary method to compute $u_1, \ldots, u_{k-1}$.

However, in the context of (8), it is natural in the variation-of-constants formula,

$$
u(t_j) = \mathrm{e}^{jhA} u_0 + \int_0^{t_j} \mathrm{e}^{(t_j - s)A} f(s, u(s))\, \mathrm{d}s, \quad 1 \le j \le k-1,
$$

to replace $f(s, u(s))$ by its Lagrange interpolation polynomial of degree $k-1$ through the nodes $\{(t_l, f(t_l, u_l))\}_{l=0}^{k-1}$. Then we are led to consider the starting approximations $u_1, \ldots, u_{k-1}$ defined by the implicit system

$$
u_j = \mathrm{e}^{jhA} u_0 + h \sum_{l=0}^{k-1} \gamma_l(j, hA) \Delta^l f_0, \quad 1 \le j \le k-1, \tag{22}
$$

which certainly possesses a unique solution $U^* = [u_1, \dots, u_{k-1}]^T$ in X_α^{k-1}. To see this, we rewrite (22) as a fixed point equation in X_α^{k-1}

$$U^* = \mathcal{N}(U^*).$$

The mapping $\mathcal{N} : X_\alpha^{k-1} \to X_\alpha^{k-1}$ is defined by

$$\mathcal{N}(W) = \xi_0 + h\Gamma(hA)F(W), \quad W = [w_1, \dots, w_{k-1}]^T,$$

where $\xi_0 = [\xi_{01}, \dots, \xi_{0,k-1}]^T \in X_\alpha^{k-1}$ has components

$$\xi_{0j} = \mathrm{e}^{jhA}u_0 + h\gamma_0(j, hA)f(0, u_0), \quad 1 \le j \le k-1,$$

$F(W) = [f(t_1, w_1), \dots, f(t_{k-1}, w_{k-1})]^T \in X^{k-1}$ and, finally, $\Gamma(hA)$ is a certain $(k-1)\times(k-1)$ operator valued matrix whose entries are linear combinations of $\gamma_l(j, hA)$, $1 \le j \le k-1$, $1 \le l \le k-1$.

Notice that (9) and (11) guarantee that $\xi_0 \in X_\alpha^{k-1}$. Moreover, by (3) and (11),

$$\|\mathcal{N}(W_2) - \mathcal{N}(W_1)\|_\alpha \le \mathcal{L}h^{1-\alpha}\|W_2 - W_1\|_\alpha,$$

where $\mathcal{L} = cLM\mathrm{e}^{\omega^* kh}$ for some $c = c(k) > 0$, which shows that $\mathcal{N}$ is a contraction for sufficiently small h.

In practice, in view of Theorem 1, it is enough to approximate U^* within the order $O(h^k)$ in the norm of X_α^{k-1}. To this end, the fixed point iteration

$$U^{[\nu+1]} = \mathcal{N}(U^{[\nu]}), \tag{23}$$

starting from a suitable $U^{[0]} = [u_1^{[0]}, \dots, u_{k-1}^{[0]}]^T \in X_\alpha^{k-1}$ can be used. Since, for $\nu \ge 1$,

$$\|U^* - U^{[\nu]}\|_\alpha \le (\mathcal{L}h^{1-\alpha})^\nu \|U^* - U^{[0]}\|_\alpha,$$

it is of interest to have $\|U^* - U^{[0]}\|_\alpha$ as small as possible. In fact, assuming that $U^{[0]}$ is chosen in such a way that

$$\|u_j^{[0]} - u(t_j)\|_\alpha \le TOL_0, \quad 1 \le j \le k-1, \tag{24}$$

we prove below that

$$\|U^* - U^{[0]}\|_\alpha \le \mathcal{C}h^{k+1-\alpha}\|g^{(k)}\|_\infty + TOL_0, \tag{25}$$

where $\mathcal{C}$ is a constant depending on k, α, L, ω, M and t_{k-1}, and $g(t) = f(t, u(t))$, $0 \le t \le t_{k-1}$.

Thus, one possibility to initialize the k-step exponential method could be:

(a) To apply some suitable auxiliary time integrator to obtain approximations $u_j^{[0]} \sim u(t_j)$, $1 \le j \le k-1$. For instance, in our numerical illustrations we use the exponential Euler method for which $TOL_0 = O(h^2)$.

(b) To use then the fixed point iteration (23) until $\|U^{[\nu+1]} - U^{[\nu]}\|_\alpha \le TOL$, with $TOL = O(h^k)$.

To prove (25), we set $\widetilde{U} = [u(t_1), \dots, u(t_{k-1})]^T \in X_\alpha^{k-1}$. Inserting $\widetilde{U}$ in (22) defines the defects $d_j \in X_\alpha$, $1 \le j \le k-1$, by

$$u(t_j) = \mathrm{e}^{jhA} u_0 + h \int_0^j \mathrm{e}^{(j-\sigma)hA} \widehat{P}_{0,k-1}(\sigma h)\, \mathrm{d}\sigma + d_j, \quad 1 \le j \le k-1,$$

where again $\widehat{P}_{0,k-1}(t)$ is the Lagrange interpolation polynomial of degree $k-1$ through the nodes $\{(t_j, g(t_j))\}_{j=0}^{k-1}$. Using (13), and proceeding as in the proof of (14), we readily obtain

$$\|d_j\|_\alpha \le c_1 M \mathrm{e}^{\omega^* kh} h^{k+1-\alpha} \|g^{(k)}\|_\infty.$$

This shows that

$$\widetilde{U} = \mathcal{N}(\widetilde{U}) + D,$$

where $D = [d_1, \dots, d_{k-1}]^T \in X_\alpha^{k-1}$ has α-norm bounded by

$$\|D\|_\alpha \le C h^{k+1-\alpha} \|g^{(k)}\|_\infty,$$

with $C = c_1 M \mathrm{e}^{\omega^* kh}$. Therefore,

$$\begin{aligned} \|U^* - \widetilde{U}\|_\alpha &\le \|\mathcal{N}(U^*) - \mathcal{N}(\widetilde{U})\|_\alpha + \|D\|_\alpha \\ &\le \mathcal{L} h^{1-\alpha} \|U^* - \widetilde{U}\|_\alpha + \|D\|_\alpha, \end{aligned}$$

which results in

$$\|U^* - \widetilde{U}\|_\alpha \le \frac{C}{1 - \mathcal{L} h^{1-\alpha}} h^{k+1-\alpha} \|g^{(k)}\|_\infty,$$

for small enough h. This estimate combined with (24), leads to (25).

5 Implementation issues

In this section we derive a recurrence for the evaluation of the entire functions $\gamma_j(k, \lambda)$, which allows us to evaluate $\gamma_j(k, h\Lambda)$ in case Λ is a diagonalizable matrix. Notice that this situation arises when the operator A itself is diagonalizable or when the Krylov approach [4,8,9] can be used.

To this end we consider the generating function

$$G(z, k, \lambda) = \sum_{j=0}^{\infty} \gamma_j(k, \lambda) z^j.$$

Since for $|z| < 1$

$$(1+z)^\sigma = \sum_{j=0}^{\infty} \binom{\sigma}{j} z^j,$$

it is clear that, for $\lambda \in \mathbf{C}$ and $|z| < 1$, we have

$$\begin{aligned} G(z,k,\lambda) &= \int_0^k \mathrm{e}^{(k-\sigma)\lambda} \left(\sum_{j=0}^{\infty} \binom{\sigma}{j} z^j \right) \mathrm{d}\sigma \\ &= \int_0^k \mathrm{e}^{(k-\sigma)\lambda} (1+z)^{\sigma} \, \mathrm{d}\sigma \\ &= \int_0^k \mathrm{e}^{(k-\sigma)\lambda + \sigma \log(1+z)} \, \mathrm{d}\sigma \\ &= \frac{(1+z)^k - \mathrm{e}^{k\lambda}}{\log(1+z) - \lambda}. \end{aligned}$$

Therefore, comparing the coefficients in the power expansions

$$(\log(1+z) - \lambda) G(z,k,\lambda) = (1+z)^k - \mathrm{e}^{k\lambda}, \tag{26}$$

we get the recursion

$$\begin{aligned} \gamma_0(k,\lambda) &= \frac{\mathrm{e}^{k\lambda} - 1}{\lambda}, \\ \gamma_j(k,\lambda) &= \frac{\left(\sum_{m=1}^{j} \frac{(-1)^{m-1}}{m} \gamma_{j-m}(k,\lambda) \right) - \binom{k}{j}}{\lambda}, \quad 1 \le j \le k, \\ \gamma_j(k,\lambda) &= \frac{\left(\sum_{m=1}^{j} \frac{(-1)^{m-1}}{m} \gamma_{j-m}(k,\lambda) \right)}{\lambda}, \quad j > k. \end{aligned} \tag{27}$$

Although (27) is meaningful as a recurrence among entire functions, it does not provide a practical way of evaluating $\gamma_j(k,0)$ and might result in a loss of accuracy for very small $|\lambda|$ (see e.g. [14]). It turns out that (26), with $\lambda = 0$, yields the analogous recursion

$$\begin{aligned} \gamma_0(k,0) &= k, \\ \gamma_j(k,0) &= \binom{k}{j+1} - \sum_{m=1}^{j} \frac{(-1)^m}{m+1} \gamma_{j-m}(k,0), \quad 1 \le j \le k-1, \\ \gamma_j(k,0) &= -\sum_{m=1}^{j} \frac{(-1)^m}{m+1} \gamma_{j-m}(k,0), \quad j > k-1. \end{aligned} \tag{28}$$

On the other hand, for very small $|\lambda|$, we could use (27) replacing the right hand sides by appropriate truncations of their Taylor expansions.

Finally, assuming that A generates a C_0-semigroup, due to the fact that the entire functions $\gamma_j(k,\lambda)$ are the Laplace transforms of measures of bounded variation, the operators $\gamma_j(k,hA)$ can also be defined by means of the Hille-Phillips holomorphic calculus [7]. This means that the derived recursion (27) remain valid at the operator level i.e. for $\lambda = hA$. Thus, in case $e^{hA}v$, $v \in X_\alpha$, is computable and a linear solver for equations $hAv = w$, $w \in X_\alpha$, is available, (27) provides a practical way of computing $\gamma_j(k, hA)v$.

6 Numerical illustration

In this section we provide numerical results obtained with the k-step exponential method (8) for $k = 2, 3, 4$. We have considered two different test problems.

The first one is the semilinear parabolic problem

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) + \left(\int_0^1 u(x,t)\,\mathrm{d}x\right)\frac{\partial u}{\partial x}(x,t) + \Phi(x,t), \tag{29}$$

for $x \in [0, 1]$ and $t \in [0, 1]$, subject to homogeneous Dirichlet boundary conditions. The source term $\Phi(x,t)$ is chosen in such a way that $u(x,t) = x(1-x)e^t$ is the exact solution of (29). This problem fits in our framework with $X = C([0, 1])$, endowed with the maximum norm, $\alpha = 1/2$ and $\omega = 0$ (see e.g. Theorem 4.3.3 in [26]).

For the spatial discretization of (29), given $J = 512$, we define the uniform grid $x_j = j/J$, $1 \le j \le J-1$. The spatial derivatives are approximated by using the standard three-point finite differences and the integral has been aproximated by using the composite Simpon's rule. In this way, since the exact solution is a polynomial of degree two in x, there are no spatial errors.

For the time integration we use (8) with $k = 2, 3, 4$, applied to the semidiscretization in space of (29). Then we have to compute $\gamma_j(k, hA)$ for the matrix $A \in \mathbf{C}^{(J-1)\times(J-1)}$,

$$A = J^2 \mathrm{tridiag}([1, -2, 1]).$$

This computation is made after diagonalizing matrix A by means of discrete Fourier techniques and using then the recurrence equations (27) obtained in Section 5. In Fig. 1 we plot errors against the step-sizes $h = 2^{-l}$, $2 \le l \le 9$. The errors are measured at each time level t_n, $k \le n \le N$, using the discrete α-norm with $\alpha = 1/2$. We observe that the slopes of the three lines are 2, 3 and 4, as expected.

The second test problem is the semilinear transport equation

$$\frac{\partial u}{\partial t}(x,t) = -\frac{\partial u}{\partial x}(x,t) + u(x,t) - u^3(x,t) + \Phi(x,t), \tag{30}$$

for $x \in [0, 1]$ and $t \in [0, 1]$, subject to periodic boundary conditions. The source term $\Phi(x,t)$ is such that $u(x,t) = e^{-t}\sin^2(\pi x) + (1 - e^{-t})$ is the exact solution of (30). This problem fits in our framework with $X = W^{1,2}([0, 1])$, $\alpha = 0$ and $\omega = 0$ [24].

Problem (30) is first approximated by a 512-point Fourier spectral discretization in x. Then, the exponential k-step method (8), with $k = 2, 3, 4$, is used for the resulting ODE system in $\mathbf{C}^J$, with $J = 512$. The application of (8) to this system of ODEs requires the evaluation of $\gamma_j(k, hA)$, where A is the spectral discretization

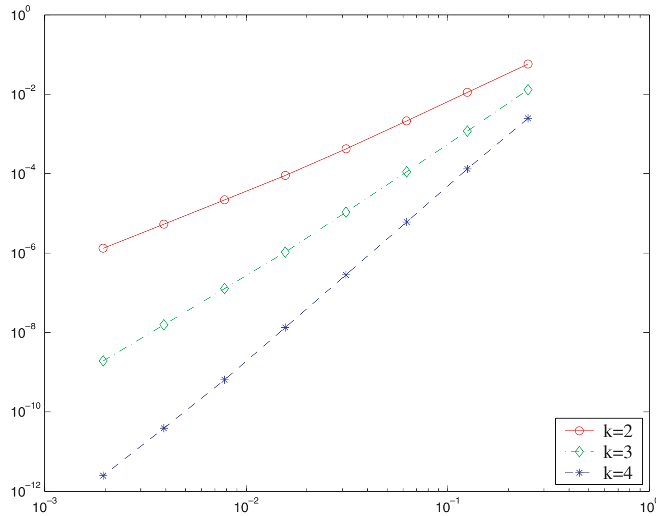

Fig. 1 Time error vs. step-size for example (29)

of $-\partial/\partial x$. In this example 0 is an eigenvalue of A. Thus, together with (27), we also need to use the recurrences (28).

Since the periodicity of u in x guarantees that the spatial error is negligible, we compute errors due to the time integration comparing with the exact solution u of (30) at the grid points. As in the previous example, these errors are measured at each time level t_n, $k \le n \le N$, using the discrete counterpart of the $W^{1,2}$-norm. In Fig. 2 again for $h = 2^{-l}$, $2 \le l \le 9$, we plot errors against the step-sizes. The plot confirms the predicted orders.

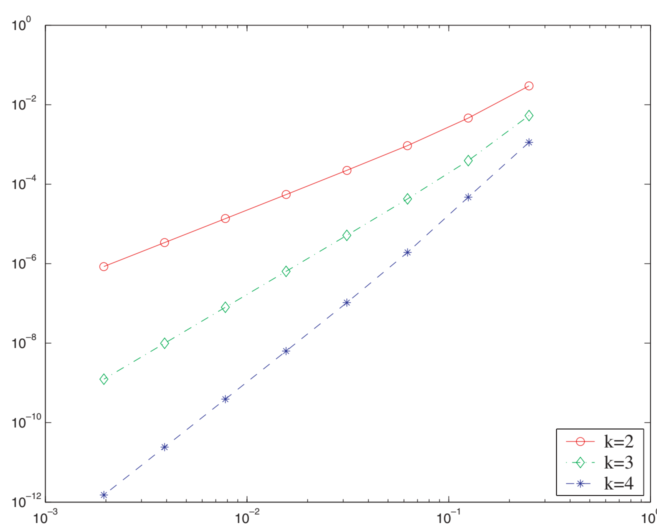

Fig. 2 Time error vs. step-size for example (30)

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