A CLASS OF EXPLICIT EXPONENTIAL GENERAL LINEAR METHODS*

A. OSTERMANN¹, M. THALHAMMER¹ and W.M. WRIGHT²

¹Institut für Mathematik, Universität Innsbruck, A-6020 Innsbruck, Austria. email: {alexander.ostermann, mechthild.thalhammer}@uibk.ac.at

²Department of Mathematical and Statistical Sciences, La Trobe University, Melbourne, Victoria 3086, Australia. email: w.wright@latrobe.edu.au

Abstract.

In this paper, we consider a class of explicit exponential integrators that includes as special cases the explicit exponential Runge–Kutta and exponential Adams–Bashforth methods. The additional freedom in the choice of the numerical schemes allows, in an easy manner, the construction of methods of arbitrarily high order with good stability properties. We provide a convergence analysis for abstract evolution equations in Banach spaces including semilinear parabolic initial-boundary value problems and spatial discretizations thereof. From this analysis, we deduce order conditions which in turn form the basis for the construction of new schemes. Our convergence results are illustrated by numerical examples.

AMS subject classification (2000): 65L05, 65L06, 65M12, 65J10.

Key words: exponential integrators, general linear methods, explicit schemes, abstract evolution equations, semilinear parabolic problems, convergence, high-order methods.

1 Introduction.

In the past few years, exponential time-integrators for semilinear problems

(1.1)
$$y'(t) = L y(t) + N(t, y(t)), \quad 0 \le t \le T, y(0)$$
 given,

have attracted a lot of interest. They are particularly appealing in situations where this differential equation comes from the spatial discretization of a partial differential equation. Exponential integrators were for the first time considered in the sixties and seventies of the last century. For a historical survey, we refer to Minchev and Wright [15].

For exponential Runge–Kutta methods, a convergence analysis for parabolic problems has recently been given by Hochbruck and Ostermann [10, 11]. The stage order for explicit schemes, however, is at most one. For that reason, the

 $[\]star$ Received August 2005. Accepted in revised form February 2006. Communicated by Timo Eirola.

construction of high-order methods is rather complicated, due to the large number of additional conditions required for stiff problems. On the other hand, the convergence of exponential Adams-type methods has been studied in Calvo and Palencia [5]. This class easily enables the construction of high-order schemes, although the resulting methods are only weakly stable in the sense that all parasitic roots for y' = 0 lie on the unit circle.

In the present paper, we are considering a class of explicit exponential integrators that combines the benefits of exponential Runge–Kutta and exponential Adams–Bashforth methods. There, it is possible to achieve high stage order which facilitates the construction of high-order methods with favorable stability properties for stiff problems. In addition, all methods included in our class are zero-stable with parasitic roots equal to zero.

An outline of the paper is as follows: In Section 2, we introduce a class of explicit exponential general linear methods based on the Adams–Bashforth schemes and further give the stage order and quadrature order conditions. These conditions form the basis for the construction of schemes of arbitrarily high order for stiff problems. In Section 3, we state our hypotheses on the problem class (1.1) employing the theory of sectorial operators in Banach spaces. In particular, parabolic initial-boundary value problems are included in our framework. The core of Section 3 is devoted to convergence estimates. Our main result is Theorem 3.4 proving that, for sufficiently smooth solutions of (1.1), the order of convergence is essentially $\min\{P, Q+1\}$. Here, P and Q denote the quadrature order and the stage order of the method, respectively. In Section 4, we exploit the order conditions in a systematic way to construct new schemes. In particular, we show that the class of two-stage methods of order p involving p-1 steps is uniquely determined up to a free parameter. Moreover, we derive a three-stage two-step method of order 4. The favorable convergence properties of our methods are illustrated in Section 5. In Section 6, we finally indicate how the convergence analysis given extends to exponential integrators with variable stepsizes.

The functions introduced below are commonly associated with *exponential* time differencing methods where the method coefficients are (linear) combinations of these functions. As we will see in Section 4, they also naturally arise in the construction of exponential general linear methods.

1.1 Exponential and related functions.

For integers $j \ge 0$ and complex numbers $z \in \mathbb{C}$, we define $\varphi_j(z)$ through

(1.2a)
$$\varphi_j(z) = \int_0^1 e^{(1-\tau)z} \frac{\tau^{j-1}}{(j-1)!} d\tau, \quad j \ge 1, \ \varphi_0(z) = e^z.$$

Consequently, the recurrence relation

(1.2b)
$$\varphi_j(z) = \frac{1}{j!} + z \,\varphi_{j+1}(z), \quad z \in \mathbb{C}, \ j \ge 0,$$

is valid.

The following result provides an expansion of the solution of a linear differential equation which is needed in the convergence analysis of Section 3.3.

LEMMA 1.1. The exact solution of the initial value problem

$$y'(t) = L y(t) + f(t), \quad t \ge t_n, y(t_n) \text{ given},$$

has the following representation

$$y(t_n + \tau) = e^{\tau L} y(t_n) + \sum_{\ell=0}^{m-1} \tau^{\ell+1} \varphi_{\ell+1}(\tau L) f^{(\ell)}(t_n) + R_n(m,\tau),$$
$$R_n(m,\tau) = \int_0^\tau e^{(\tau-\sigma)L} \int_0^\sigma \frac{(\sigma-\xi)^{m-1}}{(m-1)!} f^{(m)}(t_n+\xi) \,\mathrm{d}\xi \,\mathrm{d}\sigma, \quad \tau \ge 0,$$

provided that the function f is sufficiently many times differentiable.

PROOF. Substituting the Taylor series expansion of f

(1.3)
$$f(t_n + \sigma) = \sum_{\ell=0}^{m-1} \frac{\sigma^{\ell}}{\ell!} f^{(\ell)}(t_n) + S_n(m, \sigma),$$
$$S_n(m, \sigma) = \int_0^{\sigma} \frac{(\sigma - \xi)^{m-1}}{(m-1)!} f^{(m)}(t_n + \xi) \,\mathrm{d}\xi,$$

into the variation-of-constants formula

(1.4)
$$y(t_n + \tau) = \mathrm{e}^{\tau L} y(t_n) + \int_0^\tau \mathrm{e}^{(\tau - \sigma)L} f(t_n + \sigma) \,\mathrm{d}\sigma, \quad \tau \ge 0,$$

and applying the definition (1.2a) of the φ -functions yields the desired result.

2 Exponential general linear methods.

In this paper, we study a class of explicit exponential general linear methods that in particular contains the exponential Runge–Kutta methods and the exponential Adams-type methods considered recently in the literature, see [3, 6, 11, 12, 13] and further [5]. As will be seen from the theoretical results and the illustrations that follow in Sections 3–5, the extra freedom in the choice of the numerical method allows the construction of high-order schemes that possess favorable stability properties and exhibit no order reduction when applied to parabolic problems.

2.1 Method class.

We study explicit exponential general linear methods for the autonomous problem

(2.1)
$$y'(t) = L y(t) + N(y(t)), \quad 0 \le t \le T, y(0)$$
 given.

For given starting values $y_0, y_1, \ldots, y_{q-1}$, the numerical approximation y_{n+1} at time $t_{n+1}, n \ge q-1$, is given by the recurrence formula

(2.2a)
$$y_{n+1} = e^{hL} y_n + h \sum_{i=1}^s B_i(hL) N(Y_{ni}) + h \sum_{k=1}^{q-1} V_k(hL) N(y_{n-k}).$$

The internal stages Y_{ni} , $1 \le i \le s$, are defined through

(2.2b)
$$Y_{ni} = e^{c_i hL} y_n + h \sum_{j=1}^{i-1} A_{ij}(hL) N(Y_{nj}) + h \sum_{k=1}^{q-1} U_{ik}(hL) N(y_{n-k}).$$

The method coefficient functions $A_{ij}(hL)$, $U_{ik}(hL)$, $B_i(hL)$, and $V_k(hL)$ are linear combinations of the exponential and related φ -functions, see Section 1.1. The numerical scheme extends in an obvious way to non-autonomous problems (1.1) by replacing $N(Y_{ni})$ with $N(t_n + c_ih, Y_{ni})$ and $N(y_{n-k})$ with $N(t_{n-k}, y_{n-k})$.

The preservation of equilibria of (2.1) is guaranteed under the following conditions

(2.3)
$$\sum_{i=1}^{s} B_i(hL) + \sum_{k=1}^{q-1} V_k(hL) = \varphi_1(hL),$$
$$\sum_{j=1}^{i-1} A_{ij}(hL) + \sum_{k=1}^{q-1} U_{ik}(hL) = c_i \varphi_1(c_ihL), \quad 1 \le i \le s$$

Moreover, these conditions also ensure the equivalence of our numerical methods for autonomous and non-autonomous problems. Throughout the paper, we tacitly assume (2.3) to be satisfied. We further suppose $U_{1k}(hL) = 0$, which implies $c_1 = 0$ and thus $Y_{n1} = y_n$.

Table 2.1: The exponential general linear method (2.2) in tableau form.

c_2	$A_{21}(hL)$				$U_{21}(hL)$	 $U_{2,q-1}(hL)$
:	÷	·			÷	÷
c_s	$A_{s1}(hL)$		$A_{s,s-1}(hL)$		$U_{s1}(hL)$	 $U_{s,q-1}(hL)$
	$B_{i}(hI)$		$B_{1}(hL)$	B(hL)	$V_1(hL)$	$V_{1}(hL)$

The explicit exponential Runge–Kutta methods considered in Hochbruck and Ostermann [11], see also [6, 7, 12, 13, 19], are contained in our method class (2.2) by setting q = 1. The exponential Adams–Bashforth methods [3, 6, 16, 20] one included in (2.2) by setting s = 1.

2.2 Order conditions.

For deriving the order conditions for the method class (2.2), we assume the data in (2.1) to be sufficiently regular. In particular, we require that the nonlinearity evaluated at the exact solution f(t) = N(y(t)) is sufficiently often differentiable with respect to t for 0 < t < T.

Substituting the exact solution values

(2.4)
$$\widehat{y}_n = y(t_n), \quad \widehat{Y}_{ni} = y(t_n + c_i h), \qquad 1 \le i \le s, \ n \ge 0,$$

into the numerical scheme (2.2) defines the defects of the internal stages

(2.5a)
$$D_{ni} = \widehat{Y}_{ni} - e^{c_i h L} \, \widehat{y}_n - h \sum_{j=1}^{i-1} A_{ij}(hL) \, f(t_n + c_j h) - h \sum_{k=1}^{q-1} U_{ik}(hL) \, f(t_{n-k}), \quad 1 \le i \le s,$$

and the defect of the numerical solution

(2.5b)
$$d_{n+1} = \widehat{y}_{n+1} - e^{hL} \, \widehat{y}_n - h \sum_{i=1}^s B_i(hL) \, f(t_n + c_i h) - h \sum_{k=1}^{q-1} V_k(hL) \, f(t_{n-k}), \quad n \ge q-1.$$

We next make use of the representation for the exact solution values given in Lemma 1.1 and further expand the nonlinear term in a Taylor series, see (1.3). This leads to the following expansions for the defects of the internal stages

(2.6a)

$$D_{ni} = \sum_{\ell=1}^{Q} h^{\ell} \Theta_{\ell i}(hL) f^{(\ell-1)}(t_n) + R_{ni}^{(Q)},$$

$$\Theta_{\ell i}(hL) = c_i^{\ell} \varphi_{\ell}(c_i hL) - \sum_{j=1}^{i-1} \frac{c_j^{\ell-1}}{(\ell-1)!} A_{ij}(hL) - \sum_{k=1}^{q-1} \frac{(-k)^{\ell-1}}{(\ell-1)!} U_{ik}(hL).$$

Likewise, the numerical solution defect equals

(2.6b)
$$d_{n+1} = \sum_{\ell=1}^{P} h^{\ell} \vartheta_{\ell}(hL) f^{(\ell-1)}(t_n) + r_{n+1}^{(P)},$$
$$\vartheta_{\ell}(hL) = \varphi_{\ell}(hL) - \sum_{i=1}^{s} \frac{c_i^{\ell-1}}{(\ell-1)!} B_i(hL) - \sum_{k=1}^{q-1} \frac{(-k)^{\ell-1}}{(\ell-1)!} V_k(hL).$$

The remainders are defined through

$$R_{ni}^{(Q)} = R_n(Q, c_i h) - h \sum_{j=1}^{i-1} A_{ij}(hL) S_n(Q, c_j h)$$

$$(2.6c) \qquad -h \sum_{k=1}^{q-1} U_{ik}(hL) S_n(Q, -kh),$$

$$r_{n+1}^{(P)} = R_n(P, h) - h \sum_{i=1}^{s} B_i(hL) S_n(P, c_i h) - h \sum_{k=1}^{q-1} V_k(hL) S_n(P, -kh),$$

see Lemma 1.1 for the definition of R_n and S_n .

The numerical scheme (2.2) is said to be of stage order Q and quadrature order P if $D_{ni} = \mathcal{O}(h^{Q+1})$ for $1 \leq i \leq s$ and $d_{n+1} = \mathcal{O}(h^{P+1})$. That is, requiring $\Theta_{\ell i}(hL) = 0$ for $1 \leq i \leq s$ and $1 \leq \ell \leq Q$ as well as $\vartheta_{\ell}(hL) = 0$ for $1 \leq \ell \leq P$, we obtain the order conditions

(2.7a)

$$c_{i}^{\ell} \varphi_{\ell}(c_{i}hL) = \sum_{j=1}^{i-1} \frac{c_{j}^{\ell-1}}{(\ell-1)!} A_{ij}(hL) + \sum_{k=1}^{q-1} \frac{(-k)^{\ell-1}}{(\ell-1)!} U_{ik}(hL), \quad 1 \le i \le s, \ 1 \le \ell \le Q,$$
(2.7b)

$$\varphi_{\ell}(hL) = \sum_{i=1}^{s} \frac{c_{i}^{\ell-1}}{(\ell-1)!} B_{i}(hL) + \sum_{k=1}^{q-1} \frac{(-k)^{\ell-1}}{(\ell-1)!} V_{k}(hL), \quad 1 \le \ell \le P.$$

Here, by definition $c_i^0 = 1$ for all $1 \le i \le s$.

In Section 3, we will show that the convergence order of explicit exponential general linear methods (2.2) when applied to parabolic problems (2.1) is essentially $p = \min\{P, Q + 1\}$. Therefore, it is desirable to construct numerical schemes of high stage order.

3 Parabolic evolution equations.

In this section, we provide a convergence analysis for explicit exponential general linear methods within the framework of abstract semilinear parabolic evolution equations. For a thorough treatment of the theory of sectorial operators and analytic semigroups, we refer to the monographs [8, 14, 18].

3.1 Analytical framework.

Let X be a complex Banach space endowed with the norm $\|\cdot\|_X$ and $D \subset X$ another densely embedded Banach space. For any $0 < \vartheta < 1$ we denote by X_{ϑ} some intermediate space between $D = X_1$ and $X = X_0$ such that the norm in X_{ϑ} fulfills the relation

$$\|x\|_{X_{\vartheta}} \le C \|x\|_D^{\vartheta} \|x\|_X^{1-\vartheta}, \quad x \in D, \ 0 < \vartheta < 1,$$

414

with a constant C > 0. Examples are real interpolation spaces, see Lunardi [14], or fractional power spaces, see Henry [8].

We consider initial value problems of the form (2.1) where the right-hand side of the differential equation is defined by a linear operator $L: D \to X$ and a sufficiently regular nonlinear map

$$(3.1) N: X_{\alpha} \to X: v \mapsto N(v), \quad D \subset X_{\alpha} \subset X, \ 0 \le \alpha < 1.$$

This requirement together with Hypothesis 3.1 renders (2.1) a semilinear parabolic problem.

HYPOTHESIS 3.1. We assume that the closed and densely defined linear operator $L: D \to X$ is sectorial. Thus, there exist constants $a \in \mathbb{R}$, $0 < \phi < \pi/2$, and $M \ge 1$ such that L satisfies the resolvent condition

(3.2)
$$\|(\lambda I - L)^{-1}\|_{X \leftarrow X} \le \frac{M}{|\lambda - a|}, \quad \lambda \in \mathbb{C} \setminus S_{\phi}(a),$$

on the complement of the sector $S_{\phi}(a) = \{\lambda \in \mathbb{C} : |\arg(a - \lambda)| \leq \phi\} \cup \{a\}$. Moreover, we suppose that the graph norm of L and the norm in D are equivalent, that is, the estimate

(3.3)
$$C^{-1} \|x\|_D \le \|x\|_X + \|Lx\|_X \le C \|x\|_D, \quad x \in D,$$

is valid for a constant C > 0.

From the results in [8, 14, 18] it is well-known that the sectorial operator L is the infinitesimal generator of an analytic semigroup $(e^{tL})_{t\geq 0}$ on the underlying Banach space X. Precisely, for $L: D \to X$ sectorial and any positive t the linear operator $e^{tL}: X \to X$ is given by Cauchy's integral formula

(3.4)
$$e^{tL} = \frac{1}{2\pi i} \int_{\Gamma} e^{\lambda} (\lambda I - tL)^{-1} d\lambda, \quad t > 0,$$

with Γ denoting a path that surrounds the spectrum of L. Especially, if t = 0 one defines $e^{tL} = I$. By means of (3.2), it is shown that the estimate

(3.5)
$$||t^{\nu-\mu} e^{tL}||_{X_{\nu} \leftarrow X_{\mu}} \le C, \quad 0 \le t \le T, \ 0 \le \mu \le \nu \le 1,$$

is valid with a constant C > 0, see [14, Prop. 2.3.1]. Furthermore, for the functions defined in (1.2) the same type of bound

(3.6)
$$\left\|t^{\nu-\mu}\varphi_{\ell}(tL)\right\|_{X_{\nu}\leftarrow X_{\mu}} \le C, \quad 0 \le t \le T, \ 0 \le \mu \le \nu \le 1,$$

follows for every $\ell \geq 1$.

REMARK 3.2. Under the assumption that the nonlinear map N in (3.1) is locally Lipschitz-continuous

(3.7)
$$\|N(v) - N(w)\|_X \le C(\varrho) \|v - w\|_{X_\alpha}, \quad \|v\|_{X_\alpha} + \|w\|_{X_\alpha} \le \varrho,$$

415

the existence and uniqueness of a local solution of the semilinear parabolic problem (2.1), with initial value $y(0) \in X_{\alpha}$, is guaranteed. Moreover, the solution is represented by the variation-of-constants formula (1.4), see [8, Sect. 3.3].

The following example can be cast into our abstract framework of semilinear parabolic problems. For simplicity and in view of our numerical experiments, we restrict ourselves to one space dimension. Accordingly to Henry [8], X_{ϑ} denotes a fractional power space.

EXAMPLE 3.3. We consider the following initial-boundary value problem for a real-valued function $Y : [0,1] \times [0,T] \rightarrow \mathbb{R}$ comprising a semilinear partial differential equation subject to a homogeneous Dirichlet boundary condition and an additional initial condition

(3.8a)
$$\begin{aligned} \partial_t Y(x,t) &= \mathscr{L}(x) \, Y(x,t) + f(x,Y(x,t),\partial_x Y(x,t)), \\ Y(0,t) &= 0 = Y(1,t), \quad Y(x,0) = Y_0(x), \qquad 0 \le x \le 1, \ 0 \le t \le T. \end{aligned}$$

Here, the second-order strongly elliptic differential operator

(3.8b)
$$\mathscr{L}(x) = \alpha(x) \,\partial_{xx} + \beta(x) \,\partial_x + \gamma(x)$$

involves the coefficients $\alpha, \beta, \gamma : [0,1] \to \mathbb{R}$ which we require to be sufficiently smooth, and, in particular, $\alpha(x)$ has to be positive and bounded away from 0. Besides, we suppose the function f to be regular in all variables and to satisfy a certain growth condition in the third argument, see Henry [8, Example 3.6].

By defining a linear operator L and a map N through

$$(Lv)(x) = \mathscr{L}(x)v(x), \quad (N(v))(x) = f(x, v(x), \partial_x v(x)), \qquad v \in \mathscr{C}_0^{\infty}(0, 1),$$

the above initial-boundary value problem takes the form of an initial value problem (2.1) for (y(t))(x) = Y(x, t). The results in [8] imply that L, when considered as an unbounded operator on the Hilbert space $X = L^2(0, 1)$, satisfies Hypothesis 3.1 with $D = H^2(0, 1) \cap H^1_0(0, 1)$. Further, a suitable choice for the domain of the nonlinearity is the Sobolev space $X_{\alpha} = X_{1/2} = H^1_0(0, 1)$.

3.2 Global error relation.

Under the requirements of Section 3.1 on the initial value problem (2.1), we analyze the convergence behavior of the method class (2.2). We start with deriving a useful relation for the global error.

The errors of the numerical solution values and the internal stages, respectively, are defined through

$$e_n = \widehat{y}_n - y_n, \quad E_{ni} = \widehat{Y}_{ni} - Y_{ni}, \qquad 1 \le i \le s,$$

see (2.4). Moreover, we introduce the abbreviations

$$\Delta N_n = N(\widehat{y}_n) - N(y_n), \quad \Delta N_{ni} = N(\widehat{Y}_{ni}) - N(Y_{ni}), \qquad 1 \le i \le s.$$

Comparing formulas (2.2) and (2.5), we receive for $n \ge q-1$

(3.9a)
$$E_{ni} = e^{c_i hL} e_n + h \sum_{j=1}^{i-1} A_{ij}(hL) \Delta N_{nj} + h \sum_{k=1}^{q-1} U_{ik}(hL) \Delta N_{n-k} + D_{ni},$$

(3.9b)
$$e_{n+1} = e^{hL}e_n + h\sum_{i=1}^s B_i(hL)\Delta N_{ni} + h\sum_{k=1}^{q-1} V_k(hL)\Delta N_{n-k} + d_{n+1}.$$

Resolving the recurrence formula for e_n leads to

(3.10)
$$e_{n} = e^{(t_{n} - t_{q-1})L} e_{q-1} + \sum_{\ell=q}^{n} e^{(t_{n} - t_{\ell})L} d_{\ell} + h \sum_{\ell=q-1}^{n-1} e^{(t_{n} - t_{\ell+1})L} \times \left(\sum_{i=1}^{s} B_{i}(hL) \Delta N_{\ell i} + \sum_{k=1}^{q-1} V_{k}(hL) \Delta N_{\ell-k}\right), \quad n \ge q-1$$

In Section 3.3, we exploit the above error relation under certain requirements on the order of the method and the smoothness properties of the nonlinearity.

3.3 Convergence estimates.

Throughout, we employ the assumption that the starting values $y_0, y_1, \ldots, y_{q-1}$ have been computed using some starting procedure and that they belong to X_{α} . Further, we suppose that the method coefficients are sufficiently regular and satisfy

(3.11)
$$\begin{aligned} \|A_{ij}(hL)\|_{X_{\nu}\leftarrow X_{\mu}} + \|B_i(hL)\|_{X_{\nu}\leftarrow X_{\mu}} + \|U_{ik}(hL)\|_{X_{\nu}\leftarrow X_{\mu}} \\ + \|V_k(hL)\|_{X_{\nu}\leftarrow X_{\mu}} \le Ch^{-\nu+\mu}, \quad h > 0, \ 0 \le \mu \le \nu \le 1. \end{aligned}$$

In particular, the exponential general linear methods considered in Section 4 fulfill these requirements, see (1.2) and (3.6). As before, we set f(t) = N(y(t)) and denote $||f||_{X_{\vartheta},\infty} = \max\{||f(t)||_{X_{\vartheta}}: 0 \le t \le T\}$ for $0 \le \vartheta \le 1$.

It is straightforward to deduce the following convergence result from the global error relation (3.10).

THEOREM 3.4. Under the requirements of Hypothesis 3.1, assume that the explicit exponential general linear method (2.2) applied to the initial value problem (2.1) satisfies (3.11) and further fulfills the order conditions (2.7). Suppose that $f^{(Q)}(t) \in X_{\beta}$ for some $0 \leq \beta \leq \alpha$ and $f^{(P)}(t) \in X$. Then, for stepsizes h > 0 the estimate

$$\begin{aligned} \|y(t_n) - y_n\|_{X_{\alpha}} &\leq C \sum_{\ell=0}^{q-1} \|y(t_\ell) - y_\ell\|_{X_{\alpha}} + Ch^{Q+1-\alpha+\beta} \sup_{0 \leq t \leq t_n} \|f^{(Q)}(t)\|_{X_{\beta}} \\ &+ Ch^P \sup_{0 \leq t \leq t_n} \|f^{(P)}(t)\|_X, \quad t_q \leq t_n \leq T, \end{aligned}$$

holds with a constant C > 0 independent of n and h.

PROOF. We estimate (3.10) in the domain of the nonlinear term and obtain

$$\begin{aligned} \|e_n\|_{X_{\alpha}} &\leq \|e^{(t_n - t_{q-1})L}\|_{X_{\alpha} \leftarrow X_{\alpha}} \|e_{q-1}\|_{X_{\alpha}} + \left\|\sum_{\ell=q}^{n} e^{(t_n - t_{\ell})L} d_{\ell}\right\|_{X_{\alpha}} \\ &+ h \sum_{\ell=q-1}^{n-1} \sum_{i=1}^{s} \left\|e^{(t_n - t_{\ell+1})L} B_i(hL)\right\|_{X_{\alpha} \leftarrow X} \|\Delta N_{\ell i}\|_{X} \\ &+ h \sum_{\ell=q-1}^{n-1} \sum_{k=1}^{q-1} \left\|e^{(t_n - t_{\ell+1})L} V_k(hL)\right\|_{X_{\alpha} \leftarrow X} \|\Delta N_{\ell-k}\|_{X}. \end{aligned}$$

Consequently, using the bound (3.5) for the analytic semigroup, relation (3.11) and the Lipschitz-property (3.7), we receive

(3.12)
$$\begin{aligned} \|e_n\|_{X_{\alpha}} &\leq C \|e_{q-1}\|_{X_{\alpha}} + \left\| \sum_{\ell=q}^{n} e^{(t_n - t_{\ell})L} d_{\ell} \right\|_{X_{\alpha}} \\ &+ Ch \sum_{\ell=q-1}^{n-1} (t_n - t_{\ell})^{-\alpha} \left(\sum_{i=1}^{s} \|E_{\ell i}\|_{X_{\alpha}} + \sum_{k=1}^{q-1} \|e_{\ell-k}\|_{X_{\alpha}} \right). \end{aligned}$$

For the error of the internal stages (3.9a), measured in the norm of X_{α} , we have

$$||E_{\ell i}||_{X_{\alpha}} \leq ||e^{c_{i}hL}||_{X_{\alpha}\leftarrow X_{\alpha}}||e_{\ell}||_{X_{\alpha}} + h\sum_{j=1}^{i-1} ||A_{ij}(hL)||_{X_{\alpha}\leftarrow X} ||\Delta N_{\ell j}||_{X_{\alpha}} + h\sum_{k=1}^{q-1} ||U_{ik}(hL)||_{X_{\alpha}\leftarrow X} ||\Delta N_{\ell-k}||_{X} + ||D_{\ell i}||_{X_{\alpha}}.$$

Using again (3.5), (3.7), and (3.11), the bound

$$\|E_{\ell i}\|_{X_{\alpha}} \le C \|e_{\ell}\|_{X_{\alpha}} + Ch^{1-\alpha} \sum_{j=1}^{i-1} \|E_{\ell j}\|_{X_{\alpha}} + Ch^{1-\alpha} \sum_{k=1}^{q-1} \|e_{\ell-k}\|_{X_{\alpha}} + \|D_{\ell i}\|_{X_{\alpha}}$$

and therefore the estimate

$$||E_{\ell i}||_{X_{\alpha}} \le C ||e_{\ell}||_{X_{\alpha}} + Ch^{1-\alpha} \sum_{k=1}^{q-1} ||e_{\ell-k}||_{X_{\alpha}} + C \sum_{j=1}^{i} ||D_{\ell j}||_{X_{\alpha}}$$

follows. The constant C > 0 in particular depends on T, but is independent of h. Inserting this relation into (3.12), leads to

(3.13)
$$\begin{aligned} \|e_n\|_{X_{\alpha}} &\leq C \|e_{q-1}\|_{X_{\alpha}} + Ch \sum_{\ell=0}^{n-1} (t_n - t_{\ell})^{-\alpha} \|e_{\ell}\|_{X_{\alpha}} \\ &+ Ch \sum_{\ell=q-1}^{n-1} \sum_{i=1}^{s} (t_n - t_{\ell})^{-\alpha} \|D_{\ell i}\|_{X_{\alpha}} + \left\|\sum_{\ell=q}^{n} e^{(t_n - t_{\ell})L} d_{\ell}\right\|_{X_{\alpha}}.\end{aligned}$$

It remains to estimate the terms involving the defects (2.6). From the assumption that the stage order conditions (2.7a) are fulfilled, it follows $D_{\ell i} = R_{\ell i}^{(Q)}$ for $1 \leq i \leq s$. Therefore, provided that the Q-th order derivative of the map f is bounded in X_{β} , by (3.5) and (3.11), we obtain

$$\begin{split} \big\| R_{\ell i}^{(Q)} \big\|_{X_{\alpha}} &\leq \| R_{\ell}(Q, c_{i}h) \|_{X_{\alpha}} + h \sum_{j=1}^{i-1} \| A_{ij}(hL) \|_{X_{\alpha} \leftarrow X_{\beta}} \| S_{\ell}(Q, c_{j}h) \|_{X_{\beta}} \\ &+ h \sum_{k=1}^{q-1} \| U_{ik}(hL) \|_{X_{\alpha} \leftarrow X_{\beta}} \| S_{\ell}(Q, -kh) \|_{X_{\beta}} \\ &\leq C h^{Q+1-\alpha+\beta} \| f^{(Q)} \|_{X_{\beta},\infty}, \quad 1 \leq i \leq s, \end{split}$$

see also (2.6c) and Lemma 1.1. Moreover, the validity of the order conditions (2.7b) implies $d_{\ell} = r_{\ell}^{(P)}$. It then holds

$$\begin{aligned} \left\| r_{\ell}^{(P)} \right\|_{X} &\leq \| R_{\ell-1}(P,h) \|_{X} + h \sum_{i=1}^{s} \| B_{i}(hL) \|_{X \leftarrow X} \| S_{\ell-1}(P,c_{i}h) \|_{X} \\ &+ h \sum_{k=1}^{q-1} \| V_{k}(hL) \|_{X \leftarrow X} \| S_{\ell-1}(P,-kh) \|_{X} \\ &\leq C h^{P+1} \| f^{(P)} \|_{X,\infty}. \end{aligned}$$

Similarly, we obtain $||r_n^{(P)}||_{X_{\alpha}} \leq Ch^{P+1-\alpha} ||f^{(P)}||_{X,\infty}$. Thus, a direct estimation of the last sum in (3.13) gives

$$\sum_{\ell=q}^{(3.14)} \| \mathbf{e}^{(t_n - t_\ell)L} \|_{X_\alpha \leftarrow X} \| r_\ell^{(P)} \|_X + \| r_n^{(P)} \|_{X_\alpha} \le Ch^{P+1} \sum_{\ell=q}^{n-1} (t_n - t_\ell)^{-\alpha} \| f^{(P)} \|_{X,\infty}.$$

We insert the above estimates in (3.13) and interpret the arising sums as Riemann-sums and bound it by the corresponding integrals. From a Gronwall-type inequality with a weakly singular kernel, see [4, 17], the result follows.

The example methods given in Section 4 comprise explicit exponential general linear methods with high stage order Q = P-1. In many practical examples, the exact solution of (2.1) and the map N defining the nonlinearity are sufficiently often differentiable. That is, the assumptions $f^{(P)}(t) \in X$ and $f^{(P-1)}(t) \in X_{\alpha}$ are fulfilled for all $0 \leq t \leq T$. Therefore, the convergence order predicted by Theorem 3.4 is p = P. This result is also confirmed by the numerical examples presented in Section 5.

REMARK 3.5. Let $\alpha = 0$ and L be the generator of a \mathscr{C}_0 -semigroup, see [18]. Then, the bound $\|\varphi_j(tL)\|_{X \leftarrow X} \leq C$ is valid for finite times $0 \leq t \leq T$ and any $j \geq 0$. Returning to the above proof shows that the convergence estimate of Theorem 3.4 remains valid for \mathscr{C}_0 -semigroups with the choice $\beta = 0$. The following result shows that for parabolic problems it suffices to satisfy, instead of (2.7b), the weakened quadrature order conditions

(3.15)
$$\varphi_{\ell}(hL) = \sum_{i=1}^{s} \frac{c_i^{\ell-1}}{(\ell-1)!} B_i(hL) + \sum_{k=1}^{q-1} \frac{(-k)^{\ell-1}}{(\ell-1)!} V_k(hL), \quad 1 \le \ell \le P-1,$$
$$\frac{1}{P} = \sum_{i=1}^{s} c_i^{P-1} B_i(0) + \sum_{k=1}^{q-1} (-k)^{P-1} V_k(0),$$

to obtain the full convergence order p = P. That is, the condition where $\ell = P$ is fulfilled for L = 0, but not necessarily for arbitrary arguments, see also (1.2).

THEOREM 3.6. Assume that the requirements of Hypothesis 3.1 are valid and that the explicit exponential general linear method (2.2) fulfills (3.11). Further, suppose that the stage order conditions (2.7a) and the weak quadrature order conditions (3.15) are valid for Q = P - 1 and that $0 \le \beta \le \alpha$. Then, for stepsizes h > 0 the estimate

$$\begin{aligned} \|y(t_n) - y_n\|_{X_{\alpha}} &\leq C \sum_{\ell=0}^{q-1} \|y(t_\ell) - y_\ell\|_{X_{\alpha}} + Ch^{P-\alpha+\beta} \sup_{0 \leq t \leq t_n} \|f^{(P-1)}(t)\|_{X_{\beta}} \\ &+ Ch^P \sup_{0 \leq t \leq t_n} \|f^{(P)}(t)\|_{X}, \quad t_q \leq t_n \leq T, \end{aligned}$$

holds with a constant C > 0 independent of n and h, provided that the quantities on the right-hand side are well-defined.

PROOF. The derivation of the above result follows the lines of the proof of Theorem 3.4. For simplicity, we assume $\beta = \alpha$. It suffices to derive a refined bound for the last sum in (3.13) involving the numerical solution defects d_{ℓ} . Under the weak order conditions (3.15), the representation

$$d_{\ell} = h^{P} s_{\ell}^{(P)} + r_{\ell}^{(P)}, \quad s_{\ell}^{(P)} = \vartheta_{P}(hL) f^{(P-1)}(t_{\ell-1}),$$

is valid, see (2.6). The remainder is estimated in the same way as before and yields a contribution of $Ch^P || f^{(P)} ||_{X,\infty}$ in the convergence bound, see (3.14). We need to show that the sum

$$S = \sum_{\ell=q}^{n} \mathrm{e}^{(t_n - t_\ell)L} \, s_\ell^{(P)},$$

when measured in the norm of X_{α} , is bounded by a constant. For that purpose, we employ Abel's partial summation formula to obtain the identity

$$S = \mathscr{E}_n \, s_n^{(P)} - \mathscr{E}_{q-1} \, s_q^{(P)} - \sum_{\ell=q}^{n-1} \mathscr{E}_\ell \big(s_{\ell+1}^{(P)} - s_\ell^{(P)} \big), \quad \mathscr{E}_\ell = \sum_{j=0}^\ell \mathrm{e}^{(t_n - t_j)L}.$$

We notice that the second condition in (3.15) implies $\vartheta_P(0) = 0$, and, by Cauchy's integral formula (3.4), we further receive $\vartheta_P(hL) = hL \psi(hL)$. In particular, if the method coefficients are (linear) combinations of the φ -functions, the linear operator ψ is bounded on X. The bound

$$\begin{aligned} \|hL \,\mathscr{E}_{\ell} \,\psi(hL)\|_{X_{\nu} \leftarrow X_{\mu}} &\leq \|e^{(t_n - t_{\ell})L}\|_{X_{\nu} \leftarrow X_{\mu}} \left\|hL \,\sum_{j=0}^{\ell} e^{(t_{\ell} - t_j)L} \,\psi(hL)\right\|_{X_{\mu} \leftarrow X_{\mu}} \\ &\leq C(t_n - t_{\ell})^{-\nu + \mu}, \quad q - 1 \leq \ell < n, \ 0 \leq \mu \leq \nu < 1, \end{aligned}$$

follows by Cauchy's integral formula, see also [10, Lemma 1.1]. Further, it holds

$$\|hL \mathscr{E}_n \psi(hL)\|_{X_\nu \leftarrow X_\mu} \le C h^{-\nu+\mu}, \quad 0 \le \mu \le \nu < 1.$$

As a consequence, we obtain the estimate

$$\begin{split} \|S\|_{X_{\alpha}} &\leq \|hL \,\mathscr{E}_{n} \,\psi(hL)\|_{X_{\alpha} \leftarrow X_{\alpha}} \|f^{(P-1)}(t_{n-1})\|_{X_{\alpha}} \\ &+ \|hL \,\mathscr{E}_{q-1} \,\psi(hL)\|_{X_{\alpha} \leftarrow X_{\alpha}} \|f^{(P-1)}(t_{q-1})\|_{X_{\alpha}} \\ &+ \sum_{\ell=q}^{n-1} \|hL \,\mathscr{E}_{\ell} \,\psi(hL)\|_{X_{\alpha} \leftarrow X} \int_{0}^{h} \|f^{(P)}(t_{\ell-1} + \xi)\|_{X} \,\mathrm{d}\xi \\ &\leq C \|f^{(P-1)}\|_{X_{\alpha},\infty} + C \|f^{(P)}\|_{X,\infty} \end{split}$$

which yields the desired result.

4 Example methods.

In this section, we construct explicit exponential general linear methods (2.2) which have a favorable convergence behavior. We mainly focus on two-stage schemes with stage order Q = P - 1 where by Theorem 3.4 the full convergence order p = P is ensured for abstract evolution equations. In Section 5, the schemes are tested numerically on a semilinear parabolic initial-boundary value problem. Further, a table comparing the computational effort of various exponential integrators is included there, see Table 5.1. Among others, we count the number of evaluations of the nonlinear map N required at each step. However, by making use of the previous steps, the number of function evaluations can be reduced considerably.

Henceforth, for notational simplicity, we set z = hL and $\varphi_{ij} = \varphi_i(c_j z)$. As well, we occasionally omit the argument in the method coefficient functions and write $A_{ij} = A_{ij}(z)$ etc.

4.1 Two-stage schemes.

We first discuss explicit exponential general linear methods (2.2) with s = 2. Requiring the quadrature order and stage order conditions (2.7) to be fulfilled for q + 1 = p = P = Q + 1 determines the coefficients of the numerical scheme up to a free parameter, as the following result shows.

THEOREM 4.1. For any $0 < c_2 \leq 1$ there exists a unique explicit exponential general linear method of the form (2.2) with two stages and q steps that is convergent of order p = q + 1 for abstract parabolic problems (2.1).

PROOF. The stage order conditions (2.7a) yield the following linear equations in the unknowns A_{21} and U_{2k}

$$A_{21} + \sum_{k=1}^{p-2} U_{2k} = c_2 \varphi_{12}, \quad \sum_{k=1}^{p-2} \frac{(-k)^{\ell-1}}{(\ell-1)!} U_{2k} = c_2^{\ell} \varphi_{\ell 2}, \qquad 2 \le \ell \le p-1.$$

As this system is of Vandermonde form, it possesses a unique solution which depends on $0 < c_2 \leq 1$. Similarly, the order conditions (2.7b)

$$B_1 + B_2 + \sum_{k=1}^{p-2} V_k = \varphi_1, \quad \frac{c_2^{\ell-1}}{(\ell-1)!} B_2 + \sum_{k=1}^{p-2} \frac{(-k)^{\ell-1}}{(\ell-1)!} V_k = \varphi_\ell, \qquad 2 \le \ell \le p,$$

uniquely determine the coefficient functions B_i and V_k . By Theorem 3.4, the order of convergence for abstract evolution equations (2.1) equals p, provided that the nonlinear term f satisfies suitable regularity assumptions.

To minimize the number of φ -function evaluations, we choose to set the parameter $c_2 = 1$. The resulting methods EGLM*psq* can be considered as generalizations of the PEC schemes using an exponential Adams–Bashforth predictor of order p-1 and an exponential Adams–Moulton corrector of order p.

Order 2. To achieve order two, one has to satisfy the order conditions given in the proof of Theorem 4.1 with p = 2. To this set of equations, the uniquely determined solution is an exponential Runge–Kutta method with coefficients given in Table 4.1. The scheme EGLM221 requires three φ -function evaluations, four matrix-vector products, and two function evaluations of the nonlinear map N, provided that the values of the previous step are available.

Table 4.1: Coefficients of EGLM221 (left) and EGLM322 (right) for $c_2 = 1$.

Order 3. For convergence of order p = 3, the resulting two-stage two-step method EGLM322 requires four φ -function evaluations, six matrix-vector products, and two new function evaluations, see Table 4.1.

Order 4. The two-stage three-step method EGLM423 with coefficients given in Table 4.2 is convergent of order p = 4 and requires five φ -function evaluations, eight matrix-vector products, and two function evaluations.

Table 4.2: Coefficients of EGLM423 for
$$c_2 = 1$$
.1 $\varphi_1 + \frac{3}{2}\varphi_2 + \varphi_3$ $-2\varphi_2 - 2\varphi_3$ $\frac{1}{2}\varphi_2 + \varphi_3$ $\varphi_1 + \frac{1}{2}\varphi_2 - 2\varphi_3 - 3\varphi_4$ $\frac{1}{3}\varphi_2 + \varphi_3 + \varphi_4$ $-\varphi_2 + \varphi_3 + 3\varphi_4$ $\frac{1}{6}\varphi_2 - \varphi_4$

A MAPLE code for generating the coefficients of the schemes EGLMpsq involving s = 2 stages and q = p - 1 steps is downloadable from the webpage http://www.math.ntnu.no/num/expint/.

4.2 Schemes involving $s \geq 3$ stages.

For explicit exponential general linear methods (2.2) involving $s \geq 3$ stages, contrary to two-stage schemes, there is some freedom available in the choice of the method. This makes it feasible to suitably weight desirable properties of the numerical scheme such as stability, small error coefficients, the number of φ -function evaluations, matrix-vector products, or function evaluations. Another possibility would be to use the extra freedom available to increase the convergence order of the scheme. This involves a thorough investigation of the global error (3.10) in the lines of Hochbruck and Ostermann [11] which is beyond the scope of the present work.

For the purpose of illustration, however, we briefly describe the construction of a scheme involving s = 3 stages and q = 2 steps. For simplicity, we now assume that the nonlinear map N defining the right-hand side of the differential equation in (2.1) is defined on $X_{\alpha} = X$, see (3.1). We require the weak quadrature order conditions (3.15) and the stage order conditions (2.7a) to be fulfilled for P = 4and Q = 2. This implies that the defects of the internal stages are of the form

$$D_{ni} = h^3 \Theta_{3i}(hL) f''(t_n) + R_{ni}^{(4)},$$

$$\Theta_{3i}(hL) = c_i^3 \varphi_3(c_ihL) - \sum_{j=1}^{i-1} \frac{c_j^2}{2} A_{ij}(hL) - \frac{1}{2} U_{i1}(hL),$$

see (2.6). A suitable relation for the error of the internal stages (3.9a) together with Taylor series expansions of the nonlinearity finally shows that the error (3.10), when measured in X, is bounded by Ch^4 provided that the term

$$\sum_{i=1}^{s} B_i(hL) \, N'(y_n) \, \Theta_{3i}(hL)$$

vanishes. Altogether, the conditions for the order of convergence p = 4 with respect to the norm in X are

(4.1a)
$$\sum_{j=1}^{i-1} \frac{c_j^{\ell-1}}{(\ell-1)!} A_{ij}(hL) + \frac{(-1)^{\ell-1}}{(\ell-1)!} U_{i1}(hL) = c_i^{\ell} \varphi_{\ell}(c_i hL), \quad 1 \le \ell \le 2,$$

(4.1b)
$$\sum_{i=1}^{3} \frac{c_i^{\ell-1}}{(\ell-1)!} B_i(hL) + \frac{(-1)^{\ell-1}}{(\ell-1)!} V_1(hL) = \varphi_\ell(hL), \quad 1 \le \ell \le 3,$$

(4.1c)
$$\sum_{i=2}^{3} B_i(hL) J \Theta_{3i}(hL) = 0,$$

(4.1d)
$$\sum_{i=1}^{3} c_i^3 B_i(0) - V_1(0) = \frac{1}{4},$$

where J is an arbitrary and bounded linear operator on X.

We note that it is not possible to achieve $\Theta_{32} = 0$. Therefore, in order to satisfy condition (4.1c), we set $B_2 = \kappa B_3$ for a scalar κ . Inserting this ansatz into (4.1c) results in $B_3 J(\kappa \Theta_{32} + \Theta_{33}) = 0$. This condition can be satisfied either by setting $\kappa = 0$ or by choosing $c_2 = c_3$. In view of the computational effort required, we fulfill both which gives $B_2 = 0$ and $c_2 = c_3 = 7/10$. We refer to the resulting scheme as EGLM432. It requires eight φ -function evaluations, eight matrix-vector products, and three function evaluations.

We conclude this subsection with a brief remark on exponential generalized Runge-Kutta-Lawson methods which provided the initial motivation for considering exponential general linear methods of the form (2.2), see also [13, 15]. The basic idea for constructing these schemes is to replace the nonlinear part by an interpolation polynomial and to perform the Lawson transformation involving the exponential function. Then, a classical explicit Runge-Kutta method is used on the transformed problem and the obtained numerical solution is finally transformed back into the original variable. However, the resulting numerical schemes are inferior to methods constructed directly from the order conditions.

As an example, we mention the four-stage three-step scheme GLRK34 which satisfies the order conditions (2.7) with Q = P = 3 and the weakened quadrature order conditions (3.15) for P = 4. Thus, the order of convergence is p = 4. A MAPLE code to generate the coefficients of the generalized Lawson methods is downloadable from the website http://www.math.ntnu.no/num/expint/. The numerical experiments in Section 5 show that GLRK34 is not competitive with EGLM432 when comparing the computational effort and the size of the error.

4.3 Multistep schemes.

We conclude this section on example methods with a remark on explicit exponential multistep methods that are contained in our method class (2.2) by setting s = 1. Under the requirements q = p = P = Q + 1, the order conditions (2.7) simplify as follows

$$B_1 + \sum_{k=1}^{p-1} V_k = \varphi_1, \quad \sum_{k=1}^{p-1} (-k)^{\ell-1} V_k = (\ell-1)! \varphi_\ell, \qquad 2 \le \ell \le p,$$

and uniquely define the coefficients of the method. An alternative way for deriving these schemes is to represent the exact solution of (2.1) by means of the variation-of-constants formula

$$y(t_{n+1}) = e^{hL} y(t_n) + \int_0^h e^{(h-\tau)L} N(y(t_n+\tau)) d\tau$$

and to replace the nonlinear map N with the interpolation polynomial through the points $(t_{n-i}, N(y_{n-i}))$ for $0 \le i \le q-1$. Such exponential Adams–Bashforth methods were considered in [3, 6, 16, 20]. As an illustration, we include the four-step method EGLM414

$$y_{n+1} = e^{hL} y_n + h B_1(hL) N(y_n) + h V_1(hL) N(y_{n-1}) + h V_2(hL) N(y_{n-2}) + h V_3(hL) N(y_{n-3}),$$

with coefficient functions

$$\begin{split} B_1 &= \varphi_1 + \frac{11}{6} \,\varphi_2 + 2 \,\varphi_3 + \varphi_4, \quad V_1 &= -3 \,\varphi_2 - 5 \,\varphi_3 - 3 \,\varphi_4 \\ V_2 &= \frac{3}{2} \,\varphi_2 + 4 \,\varphi_3 + 3 \,\varphi_4, \qquad V_3 &= -\frac{1}{3} \,\varphi_2 - \varphi_3 - \varphi_4, \end{split}$$

that is convergent of order p = 4 for abstract evolution equations and requires five φ -function evaluations, five matrix-vector products, and one function evaluation.

The exponential multistep schemes studied in Calvo and Palencia [5] are instead based on the following representation of the exact solution

$$y(t_{n+1}) = e^{qhL} y(t_{n-q+1}) + \int_0^{qh} e^{(qh-\tau)L} N(y(t_{n-q+1}+\tau)) \,\mathrm{d}\tau.$$

For instance, the four-step method which we refer to as EMAM4

$$y_{n+1} = e^{4hL} y_{n-3} + h B_1(4hL) N(y_n) + h V_1(4hL) N(y_{n-1}) + h V_2(4hL) N(y_{n-2}) + h V_3(4hL) N(y_{n-3}),$$

with coefficient functions

$$\begin{split} B_1 &= \frac{16}{3}\,\varphi_2 - 64\,\varphi_3 + 256\,\varphi_4, \qquad V_1 = -\,24\,\varphi_2 + 256\,\varphi_3 - 768\,\varphi_4, \\ V_2 &= 48\,\varphi_2 - 320\,\varphi_3 + 768\,\varphi_4, \qquad V_3 = 4\,\varphi_1 - \frac{88}{3}\,\varphi_2 + 128\,\varphi_3 - 256\,\varphi_4, \end{split}$$

retains the full convergence order p = 4 for semilinear parabolic problems (2.1) and requires the same computational effort as the fourth-order scheme EGLM414.

We note that the exponential Adams–Bashforth methods are zero-stable with parasitic roots equal to zero. They have thus superior stability properties compared to the methods considered in [5] which are only weakly stable in the sense that all parasitic roots for y' = 0 lie on the unit circle.

5 Numerical experiments.

In this section, we illustrate the theoretical results given in Section 3.3 on the convergence behavior of explicit exponential general linear methods for abstract evolution equations. As a test problem, we choose a one-dimensional semilinear parabolic initial-boundary value problem.

PROBLEM 5.1 (PARABOLIC PROBLEM). We consider the following parabolic differential equation under a homogeneous Dirichlet boundary condition

$$\partial_t Y(x,t) = \partial_{xx} Y(x,t) - Y(x,t) \partial_x Y(x,t) + \Phi(x,t),$$

$$Y(0,t) = Y(1,t) = 0, \quad Y(x,0) = x(1-x), \qquad 0 \le x \le 1, \ 0 \le t \le T,$$

where Φ is chosen such that the exact solution is $Y(x,t) = x(1-x)e^t$.

As in Example 3.3, the above initial-boundary value problem is written as an abstract initial value problem of the form (1.1) for (y(t))(x) = Y(x,t) with linear operator L and nonlinearity N defined by

$$(Lv)(x) = \partial_{xx} v(x), \quad (N(t,v))(x) = -v(x) \partial_x v(x) + \Phi(x,t),$$

Table 5.1: Computational effort of various exponential integrators (order of convergence p for Problem 5.1, quadrature order P, stage order Q, number of stages s, number of steps q, number of distinct φ -functions needed to be evaluated, number of required matrix-vector products, number of (new) function evaluations of the nonlinear map N per step).

method	p	Р	Q	s	q	$\# \varphi$	#vec	#fun
EGLM221	2	2	1	2	1	3	4	2
EGLM322	3	3	2	2	2	4	6	2
EMAM4	4	4	3	1	4	5	5	1
EGLM414	4	4	3	1	4	5	5	1
EGLM423	4	4	3	2	3	5	8	2
EGLM432	$4-\gamma$	4 (weak)	2	3	2	8	8	3
ERKM4	$4-\gamma$	4 (weak)	1	5	1	8	13	5
GLRK34	4	4 (weak)	3	4	3	8	16	4

for $v \in \mathscr{C}_0^{\infty}(0, 1)$. A suitable choice for the underlying Banach space is the Hilbert space $X = L^2(0, 1)$. Then, it holds $D = H^2(0, 1) \cap H_0^1(0, 1)$ and the domain of the nonlinearity N is equal to $[0, T] \times X_{\alpha}$ where $X_{\alpha} = X_{1/2} = H_0^1(0, 1)$, see also Henry [8, Sect. 3.3].

We note that, accordingly to Lunardi [14, Sect. 7.3], an alternative choice is $X = \mathscr{C}(0,1), D = \mathscr{C}_0^2(0,1)$, and $X_{\alpha} = X_{1/2} = \mathscr{C}_0^1(0,1)$. Here, we denote $\mathscr{C}_0^k(0,1) = \{v \in \mathscr{C}^k(0,1) : v(0) = 0 = v(1)\}$ for k = 1, 2.

In order to solve Problem 5.1 numerically, we use a spatial discretization by standard finite differences of grid length $\Delta x = (M + 1)^{-1}$ with M = 200. For various explicit exponential general linear methods discussed in Section 4, the resulting system of ordinary differential equations is integrated up to time T = 1. The numerical convergence orders with respect to a discrete X_{α} -norm are determined from the exact and numerical solution values.

The numerically observed convergence orders for the explicit exponential general linear methods are in exact agreement with the values expected from the theoretical results given in Section 3.3. For example, the schemes EGLM423, EGLM414, and GLRK34 show full order p = 4, see Figures 5.1–5.2.

We point out that the scheme EGLM432 discussed in Section 4.2 and as well the exponential Runge–Kutta method ERKM4 considered in [11, Eq. (5.19)] suffer from a slight order reduction. The convergence order with respect to a discrete H_0^1 -norm is approximately $p = 4 - \gamma$ with $\gamma = 1/4$. When the error is measured in a discrete \mathscr{C}_0^1 -norm, an additional order reduction down to approximately $p = 4 - \gamma$ with $\gamma = 1/2$ is encountered. These fractional orders can be explained using arguments as in [11, Sect. 6].

In the following example, we illustrate the convergence behavior of our method class for an evolution equation which is governed by a \mathcal{C}_0 -semigroup.



Figure 5.1: The numerically observed convergence orders of various explicit exponential integrators when applied to Problem 5.1. The error measured in a discrete H_0^1 -norm is plotted versus the time stepsize.



Figure 5.2: The numerically observed convergence orders of various explicit exponential integrators when applied to Problem 5.1. The error measured in a discrete \mathscr{C}_0^1 -norm is plotted versus the time stepsize.

PROBLEM 5.2 (HYPERBOLIC PROBLEM). We consider the hyperbolic initialboundary value problem

$$\begin{split} & \mathrm{i}\,\partial_t Y(x,t) = \partial_{xx}\,Y(x,t) + \frac{1}{1+Y(x,t)^2} + \Phi(x,t), \\ & Y(0,t) = Y(1,t) = 0, \quad Y(x,0) = x(1-x), \qquad 0 \leq x \leq 1, \; 0 \leq t \leq 1, \end{split}$$

as abstract initial value problem on $X = L^2(0, 1)$. The function Φ is determined such that the exact solution equals $Y(x, t) = x(1 - x) e^t$.

As before, we use standard finite differences of grid length $\Delta x = (M + 1)^{-1}$ with M = 200 to discretize the problem in space. The obtained values for the error between the numerical and exact solution, measured in a discrete L^2 -norm, are displayed in Figure 5.3.

We note that the exact solution has bounded time derivatives of moderate size. We are therefore in the situation of Remark 3.5, and, in particular, the



Figure 5.3: The numerically observed convergence orders of various explicit exponential integrators when applied to Problem 5.2. The error measured in a discrete L^2 -norm is plotted versus the time stepsize.



Figure 5.4: The numerically observed convergence orders of the two-stage schemes EGLMp2q with q = p - 1 steps of orders $2 \le p \le 6$ when applied to Problem 5.1 (left) and Problem 5.2 (right). The error measured in a discrete \mathscr{C}_0^1 -norm and L^2 -norm, respectively, is plotted versus the time stepsize.

error bound of Theorem 3.4 applies with $\alpha = \beta = 0$. The observed convergence orders confirm the theoretically predicted values.

We conclude this section with an additional numerical experiment where we illustrate the error behavior of the exponential methods EGLM*psq* with s = 2 stages and q = p - 1 steps of order p for the above test problems, see Figure 5.4.

Due to the special structures of the above test problems, Fourier techniques are applicable for the numerical implementation of the φ -functions. We therefore used this approach in our numerical experiments. In more general situations where spectral techniques do not apply, matrix functions can be computed by subspace methods such as Krylov subspace techniques, see [9] and references cited therein. If the dimension of the involved matrices is moderate, an alternative implementation of the φ -functions is provided by the MATLAB package [2], downloadable from the website http://www.math.ntnu.no/num/expint/.

6 Extension to variable stepsizes.

In this section, we briefly indicate how the techniques employed in this paper extend to variable stepsizes.

We let $(h_j)_{j\geq 0}$ be a sequence of positive stepsizes and define the associated grid points through $t_{j+1} = t_j + h_j$ for $j \geq 0$, where $t_0 = 0$. The stepsize ratios $(\omega_j)_{j\geq 1}$ are given by $h_j = \omega_j h_{j-1}$. As described in Section 4.3, a generic tool for the construction of numerical methods for (2.1) is the variation-of-constants formula

(6.1)
$$y(t_{n+1}) = e^{h_n L} y(t_n) + \int_0^{h_n} e^{(h_n - \tau)L} N(y(t_n + \tau)) \, \mathrm{d}\tau,$$

together with a replacement of the nonlinear term by some interpolation polynomial.

To keep the presentation simple, we illustrate the basic ideas by an explicit exponential integrator involving two stages and two steps. This generalizes the scheme EGLM322 of Section 4.1 to variable stepsizes. In order to determine the internal stage Y_{n2} , we replace N in (6.1) with the polynomial through $(t_{n-1}, N(y_{n-1}))$ and $(t_n, N(y_n))$. Integration yields

$$Y_{n2} = e^{h_n L} y_n + h_n A_{21}^{(n)}(h_n L) N(y_n) + h_n U_{21}^{(n)}(h_n L) N(y_{n-1}),$$
$$A_{21}^{(n)} = \varphi_1 + \omega_n \varphi_2, \quad U_{21}^{(n)} = -\omega_n \varphi_2.$$

Similarly, we obtain the numerical solution value

$$y_{n+1} = e^{h_n L} y_n + h_n B_1^{(n)}(h_n L) N(y_n) + h_n B_2^{(n)}(h_n L) N(Y_{n2}) + h_n V_1^{(n)}(h_n L) N(y_{n-1}), B_1^{(n)} = A_{21}^{(n)} - (\varphi_2 + 2\omega_n \varphi_3), \quad B_2^{(n)} = \frac{1}{1 + \omega_n} (\varphi_2 + 2\omega_n \varphi_3), V_1^{(n)} = U_{21}^{(n)} + \frac{\omega_n}{1 + \omega_n} (\varphi_2 + 2\omega_n \varphi_3),$$

by interpolating through the above points and $(t_{n+1}, N(Y_{n2}))$.

More generally, we allow explicit exponential general linear methods with coefficients depending on several subsequent stepsize ratios

$$y_{n+1} = e^{h_n L} y_n + h_n \sum_{i=1}^s B_i^{(n)}(h_n L) N(Y_{ni}) + h_n \sum_{k=1}^{q-1} V_k^{(n)}(h_n L) N(y_{n-k}),$$
$$Y_{ni} = e^{c_i h_n L} y_n + h_n \sum_{j=1}^i A_{ij}^{(n)}(h_n L) N(Y_{nj}) + h_n \sum_{k=1}^{q-1} U_{ik}^{(n)}(h_n L) N(y_{n-k}),$$

see also (2.2). Provided that the stepsize ratios are bounded from above and below, that is, it holds

(6.2)
$$C_1 \le \omega_j \le C_2, \quad j \ge 1,$$

with (moderate) constants $C_1, C_2 > 0$, the coefficient operators satisfy an estimate of the form (3.11) with h replaced by h_n . We emphasize that assumption (6.2) is always fulfilled in practical implementations. Due to the special form of the considered method class, no further requirements on the stepsize sequence are needed. As a consequence, it is straightforward to generalize the convergence analysis of Section 3.3. More precisely, by means of a Gronwall-type inequality derived in Bakaev [1, Lemma 4.4], the proof of Theorem 3.4 extends literally to variable stepsizes. We do not elaborate the details here.

7 Conclusions.

The present work shows that the considered class of exponential integrators has the following benefits. It allows, in an easy manner, the construction of methods with high stage order and excellent convergence properties for stiff problems. Further, the combination of exponential Runge–Kutta and exponential Adams– Bashforth methods results in schemes with favorable stability properties.

It is beyond the scope of this paper to identify methods which are competitive with established schemes. To reach this aim, it is indispensable to implement the method with variable stepsizes based on an error control. In particular, an efficient implementation of the φ -functions plays a crucial role here. Also, it remains to look into the computation of the starting values. These investigations are part of future work.

Acknowledgement.

Mechthild Thalhammer was supported by Fonds zur Förderung der wissenschaftlichen Forschung (FWF) under project H210-N13.

REFERENCES

- N. Y. Bakaev, On variable stepsize Runge-Kutta approximations of a Cauchy problem for the evolution equation, BIT, 38 (1998) pp. 462–485.
- H. Berland, B. Skaflestad, and W. M. Wright, Expint A Matlab package for exponential integrators, Tech. report 4/05, Department of Mathematics, NTNU, 2005.
- G. Beylkin, J. M. Keiser, and L. Vozovoi, A new class of time discretization schemes for the solution of nonlinear PDEs, J. Comput. Phys., 147 (1998), pp. 362–387.
- H. Brunner and P. J. van der Houwen, The Numerical Solution of Volterra Equations, CWI Monographs 3, North-Holland, Amsterdam, 1986.
- M. P. Calvo and C. Palencia, A class of explicit multistep exponential integrators for semilinear problems, Numer. Math., 102 (2006), pp. 367–381.
- P. M. Cox and P. C. Matthews, Exponential time differencing for stiff systems, J. Comput. Phys., 176 (2002), pp. 430–455.
- A. Friedli, Verallgemeinerte Runge-Kutta Verfahren zur Lösung steifer Differentialgleichungssysteme, in Numerical Treatment of Differential Equations, R. Bulirsch, R. Grigorieff, and J. Schröder, (eds.), Lecture Notes in Mathematics, vol. 631, pp. 35–50, Springer, Berlin, 1978.

- D. Henry, Geometric Theory of Semilinear Parabolic Equations, Lecture Notes in Mathematics, vol. 840, Springer, Berlin, 1981.
- 9. M. Hochbruck and M. E. Hochstenbach, Subspace extraction for matrix functions, preprint, Department of Mathematics, Case Western Reserve University, 2005.
- M. Hochbruck and A. Ostermann, Exponential Runge-Kutta methods for parabolic problems, Appl. Numer. Math., 53 (2005), pp. 323–339.
- M. Hochbruck and A. Ostermann, Explicit exponential Runge-Kutta methods for semilinear parabolic problems, SIAM J. Numer. Anal., 43 (2005), pp. 1069–1090.
- A. K. Kassam and L. N. Trefethen, Fourth-order time stepping for stiff PDEs, SIAM J. Sci. Comput., 26 (2005), pp. 1214–1233.
- S. Krogstad, Generalized integrating factor methods for stiff PDEs, J. Comput. Phys., 203 (2005), pp. 72–88.
- 14. A. Lunardi, Analytic Semigroups and Optimal Regularity in Parabolic Problems, Birkhäuser, Basel, 1995.
- B. V. Minchev and W. M. Wright, A review of exponential integrators for first order semi-linear problems, Tech. report 2/05, Department of Mathematics, NTNU, 2005.
- S. P. Nørsett, An A-stable modification of the Adams-Bashforth methods, in Conference on the Numerical Solution of Differential Equations, J. Morris, ed., Lecture Notes in Mathematics, vol. 109, pp. 214–219, Springer, Berlin, 1969.
- A. Ostermann and M. Thalhammer, Non-smooth data error estimates for linearly implicit Runge-Kutta methods, IMA J. Numer. Anal., 20 (2000), pp. 167–184.
- A. Pazy, Semigroups of Linear Operators and Applications to Partial Differential Equations, Springer, New York, 1983.
- K. Strehmel and R. Weiner, B-convergence results for linearly-implicit one step methods, BIT, 27 (1987), pp. 264–281.
- J. G. Verwer, On generalized linear multistep methods with zero-parasitic roots and an adaptive principal root, Numer. Math., 27 (1977), pp. 143–155.