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Exponential multistep methods of Adams-type

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Abstract The paper is concerned with the construction, implementation and numerical analysis of exponential multistep methods. These methods are related to explicit Adams methods but, in contrast to the latter, make direct use of the exponential and related matrix functions of a (possibly rough) linearization of the vector field. This feature enables them to integrate stiff problems explicitly in time.

A stiff error analysis is performed in an abstract framework of linear semigroups that includes semilinear evolution equations and their spatial discretizations. A possible implementation of the proposed methods, including the computation of starting values and the evaluation of the arising matrix functions by Krylov subspace methods is discussed. Moreover, an interesting connection between exponential Adams methods and a class of local time stepping schemes is established.

Numerical examples that illustrate the methods' properties are included.

Keywords exponential integrators · exponential Adams methods · linearized exponential multistep methods · evolution equations · local time stepping

Mathematics Subject Classification (2000) 65L20 · 65L06 · 65J10 · 65M12

1 Introduction

In this paper we are concerned with the construction, implementation and numerical analysis of exponential multistep methods for stiff initial value problems of the general form

$$u'(t) = F\big(t, u(t)\big), \qquad u(t_0) = u_0. \tag{1.1}$$

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Our main interest lies in abstract evolution equations like parabolic initial boundary value problems or spatial discretizations thereof. As in all exponential integrators, the formulation of the method relies on an appropriate linearization of the vector field and employs the exponential and related function of this linearization. We will distinguish two different cases throughout the paper, namely integrators for semilinear problems and integrators that are based on a continuous linearization.

We start off with semilinear problems of the form

$$u'(t) = -Au(t) + g\big(t, u(t)\big), \qquad u(t_0) = u_0 \tag{1.2}$$

which arise from (1.1) by identifying a dominant stiff part. The nonlinear remainder g is assumed to satisfy a local Lipschitz condition with a moderate Lipschitz constant. In practise, the form (1.2) can be obtained from (1.1) by a (rough) linearization at a certain state, e.g. at the initial state. For the numerical solution of (1.2), we consider the class of so-called exponential Adams methods, first introduced by Certaine [2] and in a more systematic way by Nørsett [14]. The main contribution of our paper is a rigorous error analysis for these methods. Note that Calvo and Palencia [1] constructed and analyzed a related class of k-step methods, where the variation-of-constants formula is taken over an interval of length kh instead of h. In contrast to exponential Adams methods, all parasitic roots of their methods are on the unit circle.

As a second class of methods, we consider exponential multistep methods which are based on a continuous linearization of the vector field along the numerical trajectory. These methods enjoy the property that the nonlinearity, which is integrated explicitly in time, has a very small Lipschitz constant (actually being zero at the beginning of each step). Therefore, these methods admit larger time steps, in general. The first method of this type appeared in a paper by Pope [17], a two-step scheme was proposed more recently by Tokman [18]. She also raised the question about the existence of higher-order methods of this type. We present here a general class of linearized exponential multistep methods which is based on interpolation with a Hermite node at the beginning of each step. For both kind of methods, we propose starting procedures which are inspired by a construction in [1].

The error analysis for our methods is carried out in an abstract Banach space framework of linear semigroups. We work under the assumption that $-A$ generates an analytic semigroup and that the nonlinear remainder g is locally Lipschitz continuous. Such an assumption is typically fulfilled for parabolic initial boundary value problems and their spatial discretizations. We note that our analysis can also be carried out for strongly continuous semigroups. We show that the k-step exponential Adams method converges with order k, whereas the linearized k-step exponential Adams method is shown to converge with order $k+1$. These high-order convergence properties are illustrated by numerical experiments.

Exponential Adams method are a special case of exponential general linear methods, for which an error analysis based on order conditions can be found in [15]. The analysis presented in the current paper is in the spirit of traditional convergence proofs for multistep methods. This is conceptually simpler and can easily be generalized to linearized methods.

For the implementation of exponential multistep methods, we consider multiple time stepping techniques and Krylov subspace methods. For the latter purpose, it is advisable to rewrite the (linearized) exponential Adams method as a perturbation of the (linearized) exponential Euler method. The Krylov approximations then become increasingly cheaper for each additional backward difference. We illustrate this property by a numerical experiment.

We conclude our paper by establishing an interesting connection between explicit local time stepping and exponential Adams methods. It turns out that the explicit local time stepping method of [5] can be interpreted as a particular implementation of an exponential Adams method, where small time steps are used to approximate the arising matrix functions.

2 Exponential Adams methods

Throughout this section we write the right-hand side F of (1.1) as

$$F\big(t,u\big) = -Au + g(t,u) \tag{2.1}$$

with a certain matrix (or linear operator) A. Such a representation can be achieved by linearizing the function at a certain state, for instance at the initial value u_0.

Formally, the exact solution of (1.1) then satisfies the variation-of-constants formula

$$u(t_{n+m}) = \mathrm{e}^{-mhA}u(t_n) + \int_0^{mh} \mathrm{e}^{-(mh-\tau)A} g\big(t_n+\tau, u(t_n+\tau)\big)\mathrm{d}\tau \tag{2.2}$$

for $m \geq 0$. The derivation of the numerical method proceeds in the same way as for explicit Adams methods. Given approximations $u_j \approx u(t_j)$, we consider the interpolation polynomial p_n through the points

$$\big(t_{n-k+1}, g(t_{n-k+1}, u_{n-k+1})\big), \ldots, \big(t_n, g(t_n,u_n)\big),$$

given by

$$p_n(t_n+\theta h) = G_n + \sum_{j=1}^{k-1} (-1)^j \binom{-\theta}{j} \nabla^j G_n, \quad G_j = g(t_j,u_j). \tag{2.3}$$

Here, $\nabla^j G_n$ denotes the jth backward difference, defined recursively by

$$\nabla^0 G_n = G_n, \quad \nabla^j G_n = \nabla^{j-1}G_n - \nabla^{j-1}G_{n-1}, \quad j = 1,2,\ldots.$$

Replacing the nonlinearity g_n in (2.2) with $m=1$ by the interpolation polynomial p_n defines the numerical method

$$u_{n+1} = \mathrm{e}^{-hA}u_n + \int_0^h \mathrm{e}^{-(h-\tau)A} p_n(t_n+\tau)\mathrm{d}\tau. \tag{2.4}$$

By inserting the interpolation polynomial into (2.4), we get the scheme

$$u_{n+1} = u_n + h\varphi_1(-hA)F(t_n,u_n) + h\sum_{j=1}^{k-1} \gamma_j(-hA)\nabla^j G_n \tag{2.5a}$$

with weights $\varphi_1(z) = \gamma_0(z)$ and

$$\gamma_j(z) = (-1)^j \int_0^1 \mathrm{e}^{(1-\theta)z} \binom{-\theta}{j} \mathrm{d}\theta, \qquad j \geq 0. \tag{2.5b}$$

We call (2.5) henceforth *(explicit) exponential Adams methods*. Note that the methods make explicit use of (matrix) functions of A. For $A = 0$ the exponential Adams methods reduce to the well-known classical explicit Adams methods, see, e.g., [8, Chapter III]. Exponential multistep methods were first introduced in [2] and then generalized in [14]. The same class of methods was rediscovered much later in [3]. In all of theses papers, a rigorous error analysis for stiff problems is missing. Related methods using rational approximation of the arising matrix functions are presented in [13] and [19].

In terms of φ-functions

$$\varphi_j(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} \frac{\theta^{j-1}}{(j-1)!} \mathrm{d}\theta, \qquad j \geq 1,$$

the weights of exponential Adams methods are given by

$$\begin{aligned}
\gamma_1 &= \varphi_2, \\
\gamma_2 &= \varphi_3 + \tfrac{1}{2}\varphi_2, \\
\gamma_3 &= \varphi_4 + \varphi_3 + \tfrac{1}{3}\varphi_2, \\
\gamma_4 &= \varphi_5 + \tfrac{3}{2}\varphi_4 + \tfrac{11}{12}\varphi_3 + \tfrac{1}{4}\varphi_2, \\
\gamma_5 &= \varphi_6 + 2\varphi_5 + \tfrac{7}{4}\varphi_4 + \tfrac{5}{6}\varphi_3 + \tfrac{1}{5}\varphi_2.
\end{aligned}$$

Example 2.1 For $k = 1$ we obtain the exponential Euler method

$$u_{n+1} = u_n + h\varphi_1(-hA)F(t_n, u_n), \tag{2.6}$$

while for $k = 2$ we have

$$u_{n+1} = u_n + h\varphi_1(-hA)F(t_n, u_n) + h\varphi_2(-hA)(G_n - G_{n-1}), \tag{2.7}$$

which will be seen to be second-order convergent.

Note that (2.5a) can be interpreted as a corrected exponential Euler step. If the implementation of the products of the weights $\gamma_j(-hA)$ and the backward differences $\nabla^j G_n$ is done with Krylov subspace methods, then the Euler step turns out to be the most expensive part. Our error analysis below shows that $\|\nabla^j G_n\| = O(h^j)$ for sufficiently smooth solutions, so it can be expected that Krylov approximations become cheaper with increasing j; see also [18].

It was proposed in [1] to define starting approximations $u_1, \ldots, u_{k-1}$ by replacing the nonlinearity in (2.2) by the polynomial

$$p(t_0 + \theta h) = G_0 + \sum_{\ell=1}^{k-1} \binom{\theta}{\ell} \Delta^\ell G_0$$

interpolating in $\big(t_0, g(t_0,u_0)\big), \ldots, \big(t_{k-1}, g(t_{k-1},u_{k-1})\big)$. Here $\Delta^j G_0$ denotes the jth forward difference defined recursively by

$$\Delta^0 G_n = G_n, \qquad \Delta^j G_n = \Delta^{j-1} G_{n+1} - \Delta^{j-1} G_n, \qquad j = 1,2,\ldots.$$

Approximations $u_1, \ldots, u_{k-1}$ of appropriate order are obtained by solving the nonlinear system

$$u_m = u_0 + mh\varphi_1(-mhA)F(t_0,u_0) + h\sum_{\ell=1}^{k-1} \sigma_{m,\ell}(-hA)\Delta^\ell G_0, \qquad m = 1,\ldots,k-1, \tag{2.8}$$

where

$$\sigma_{m,\ell}(z) = \int_0^m \mathrm{e}^{(m-\theta)z} \binom{\theta}{\ell} \mathrm{d}\theta.$$

A comparison with (2.5b) yields

$$\begin{aligned}
\sigma_{m,1}(z) &= m^2\varphi_2(mz),\\
\sigma_{m,2}(z) &= m^3\varphi_3(mz) - \tfrac{1}{2}m^2\varphi_2(mz),\\
\sigma_{m,3}(z) &= m^4\varphi_4(mz) - m^3\varphi_3(mz) + \tfrac{1}{3}m^2\varphi_2(mz),\\
\sigma_{m,4}(z) &= m^5\varphi_5(mz) - \tfrac{3}{2}m^4\varphi_4(mz) + \tfrac{11}{12}m^3\varphi_3(mz) - \tfrac{1}{4}m^2\varphi_2(mz),\\
\sigma_{m,5}(z) &= m^6\varphi_6(mz) - 2m^5\varphi_5(mz) + \tfrac{7}{4}m^4\varphi_4(mz) - \tfrac{5}{6}m^3\varphi_3(mz) + \tfrac{1}{5}m^2\varphi_2(mz).
\end{aligned}$$

Note that, up to the alternating sign, the coefficients of $\sigma_{1,j}$ coincide with those for $\gamma_j(z)$. This can be easily verified from the definition of these functions.

Under appropriate assumptions (see Section 4 below), the nonlinear system (2.8) has a unique solution $(u_1,\ldots,u_{k-1})$ for h sufficiently small. The solution can be computed by fixed point iteration, cf. [1, Section 4].

3 Linearized exponential multistep methods

The numerical schemes considered so far are based on a single linearization of the right-hand side F. Next we construct methods based on a continuous linearization of (1.1) along the numerical solution. For a given point u_n approximating $u(t_n)$, we define

$$J_n = \frac{\partial F}{\partial u}(t_n,u_n), \quad d_n = \frac{\partial F}{\partial t}(t_n,u_n), \quad g_n(t,u) = F(t,u) - J_n u - d_n t. \tag{3.1}$$

The numerical schemes given below will make *explicit* use of these quantities. In the above notation, (1.1) takes the form

$$u'(t) = J_n u(t) + d_n t + g_n\big(t,u(t)\big). \tag{3.2}$$

The variation-of-constants formula thus yields the following representation of the exact solution for $m \ge 0$

$$u(t_{n+m}) = \mathrm{e}^{mhJ_n}u(t_n) + \int_0^{mh} \mathrm{e}^{(mh-\tau)J_n}\big((t_n+\tau)d_n + g_n\big(t_n+\tau, u(t_n+\tau)\big)\big)\,\mathrm{d}\tau. \tag{3.3}$$

In contrast to exponential Adams methods, we can now exploit the relations

$$\frac{\partial g_n}{\partial u}(t_n,u_n)=0, \qquad \frac{\partial g_n}{\partial t}(t_n,u_n)=0 \tag{3.4}$$

by approximating g_n in (3.3) by a Hermite interpolation polynomial $\widehat{p}_n$ of degree k satisfying $\widehat{p}_n'(t_n)=0$ and interpolating in the points

$$\big(t_{n-k+1},g_n(t_{n-k+1},u_{n-k+1})\big),\dots,\big(t_n,g_n(t_n,u_n)\big).$$

This polynomial is given by

$$\widehat{p}_n(t_n+\theta h)=G_{n,n}+\sum_{j=1}^{k-1}(-1)^{j+1}\theta\binom{-\theta}{j}\sum_{\ell=1}^{j}\tfrac{1}{\ell}\nabla^\ell G_{n,n}, \tag{3.5}$$

where $G_{n,m}=g_n(t_m,u_m)$ and $\nabla^j G_{n,m}$ denotes the jth backward difference defined recursively by

$$\nabla^0 G_{n,m}=G_{n,m}, \qquad \nabla^j G_{n,m}=\nabla^{j-1}G_{n,m}-\nabla^{j-1}G_{n,m-1}, \qquad j=1,2,\dots. \tag{3.6}$$

Replacing g_n in (3.3) by this polynomial defines the numerical scheme

$$\begin{aligned} u_{n+1} &= \mathrm{e}^{hJ_n}u_n+h\int_0^1 \mathrm{e}^{h(1-\theta)J_n}\big((t_n+\theta h)d_n+\widehat{p}_n(t_n+\theta h)\big)\,\mathrm{d}\theta \qquad (3.7a)\\ &= u_n+h\varphi_1(hJ_n)F(t_n,u_n)+h^2\varphi_2(hJ_n)d_n+h\sum_{j=1}^{k-1}\widehat{\gamma}_{j+1}(hJ_n)\sum_{\ell=1}^{j}\tfrac{1}{\ell}\nabla^\ell G_{n,n} \end{aligned}$$

which we call *linearized exponential Adams method* henceforth. Its weights

$$\widehat{\gamma}_{j+1}(z)=(-1)^{j+1}\int_0^1 \mathrm{e}^{(1-\theta)z}\theta\binom{-\theta}{j}\mathrm{d}\theta \tag{3.7b}$$

expressed in terms of φ-functions are

$$\begin{aligned} \widehat{\gamma}_2&=-2\varphi_3,\\ \widehat{\gamma}_3&=-3\varphi_4-\varphi_3,\\ \widehat{\gamma}_4&=-4\varphi_5-3\varphi_4-\tfrac{2}{3}\varphi_3,\\ \widehat{\gamma}_5&=-5\varphi_6-6\varphi_5-\tfrac{11}{4}\varphi_4-\tfrac{1}{2}\varphi_3. \end{aligned}$$

Example 3.1 For $k=1$ we obtain the *linearized exponential Euler method* (also called *exponential Rosenbrock–Euler method*)

$$u_{n+1}=u_n+h\varphi_1(hJ_n)F(t_n,u_n)+h^2\varphi_2(hJ_n)d_n, \tag{3.8}$$

which is second-order convergent. For $k=2$ we get third-order scheme

$$u_{n+1}=u_n+h\varphi_1(hJ_n)F(t_n,u_n)+h^2\varphi_2(hJ_n)d_n-2h\varphi_3(hJ_n)(G_{n,n}-G_{n,n-1}) \tag{3.9}$$

which was first presented in [11].

Motivated by the approach in [1], we suggest to construct starting values by replacing the nonlinearity g_n in (3.3) by the interpolation polynomial

$$\widehat{p}(t_0+\theta h) = G_{0,0} + \sum_{j=1}^{k-1} (-1)^j \theta \binom{\theta}{j} \sum_{\ell=1}^{j} (-1)^\ell \tfrac{1}{\ell} \Delta^\ell G_{0,0}$$

satisfying $\widehat{p}'(t_0) = 0$ and interpolating in

$$\big(t_0, g_0(t_0,u_0)\big), \ldots, \big(t_{k-1}, g_0(t_{k-1},u_{k-1})\big).$$

Here, the forward differences are defined analogously to (3.6). The approximations $u_1, \ldots, u_{k-1}$ are obtained by solving the nonlinear system

$$\begin{aligned} u_m = u_0 &+ (mh)\varphi_1(mhJ_0)F(t_0,u_0) + (mh)^2\varphi_2(mhJ_0)d_0 \\ &+ h\sum_{j=1}^{k-1} \widehat{\sigma}_{m,j}(hJ_0) \sum_{\ell=1}^{j} \frac{(-1)^\ell}{\ell} \Delta^\ell G_{0,0}, \qquad m = 1, \ldots, k-1, \end{aligned} \tag{3.10}$$

where

$$\widehat{\sigma}_{m,j}(z) = (-1)^j \int_0^m \mathrm{e}^{(m-\theta)z} \theta \binom{\theta}{j} \mathrm{d}\theta.$$

A straightforward calculation shows that

$$\begin{aligned} \widehat{\sigma}_{m,1}(z) &= -2m^3\varphi_3(mz), \\ \widehat{\sigma}_{m,2}(z) &= 3m^4\varphi_4(mz) - m^3\varphi_3(mz), \\ \widehat{\sigma}_{m,3}(z) &= -4m^5\varphi_5(mz) + 3m^4\varphi_4(mz) - \tfrac{2}{3}m^3\varphi_3(mz), \\ \widehat{\sigma}_{m,4}(z) &= 5m^6\varphi_6(mz) - 6m^5\varphi_5(mz) + \tfrac{11}{4}m^4\varphi_4(mz) - \tfrac{1}{2}m^3\varphi_3(mz). \end{aligned}$$

Note that, up to the alternating sign, the coefficients of $\widehat{\sigma}_{1,j}$ coincide with those for $\widehat{\gamma}_j(z)$. This can be easily verified from the definition of these functions.

For h sufficiently small, the nonlinear system (3.10) has a unique solution which can be approximated by fixed point iteration.

4 Error analysis

So far, we have considered a finite dimensional setting with A being a square matrix. The main ingredients for the construction of our schemes where the variation-of-constants formula and the possibility to define appropriate matrix functions.

The purpose of this section is to give an error analysis for stiff problems. We will derive uniform error bounds on bounded time intervals. The bounds are of the form Ch^p, where the constant C is independent of the stiffness of the problem and the employed time step size h. Throughout this section, $C > 0$ will denote a generic constant.

An appropriate framework for carrying out this analysis are semigroups of linear operators. We will therefore make the following assumptions, for more details, we refer to [4, 9, 16].

Assumption 4.1 *Let X be a Banach space with norm $\|\cdot\|$. We assume that A is a linear operator on X and that $(-A)$ is the infinitesimal generator of an analytic semigroup e^{-tA} on X.* ○

Without loss of generality, we assume that the sector containing the spectrum of A is bounded away from the origin. In this case, the fractional powers of A are well defined. For a fixed α with $0 \le \alpha < 1$, let

$$V = \{v \in X \mid A^\alpha v \in X\} \subset X.$$

Then V is a Banach space with norm $\|v\|_V = \|A^\alpha v\|$ which is equivalent to the graph norm of A^α. Recall that under the above assumptions, the following parabolic smoothing property holds:

$$\|\mathrm{e}^{-tA}\|_{X\leftarrow X} + \|t^\gamma A^\gamma \mathrm{e}^{-tA}\|_{X\leftarrow X} \le C_\gamma, \qquad \gamma, t \ge 0. \tag{4.1}$$

Our main assumption on the nonlinearity will be the following.

Assumption 4.2 *We assume that $g : [0,T] \times V \to X$ is locally Lipschitz-continuous in a strip along the exact solution u.* ○

Recall that this framework covers semilinear parabolic equations, such as reaction-diffusion equations, and their spatial discretizations. For more details, we refer to [9, Chapter 3].

4.1 Convergence of exponential Adams methods

We are now in the position to state our main convergence result for exponential Adams methods.

Theorem 4.3 *Let the initial value problem* (1.2) *satisfy Assumptions 4.1 and 4.2, and consider for its numerical solution the k-step exponential Adams method* (2.5) *with step size h satisfying $0 < h \le H$ with H sufficiently small. Let $f(t) = g\big(t, u(t)\big)$ and assume that $f \in C^k([0,T], X)$. Then, for*

$$\big\|u_j - u(t_j)\big\|_V \le c_0 h^k, \quad j = 1, \dots, k-1, \tag{4.2}$$

the error bound

$$\|u_n - u(t_n)\|_V \le C \cdot h^k \sup_{0\le t\le t_n} \|f^{(k)}(t)\|$$

holds uniformly in $0 \le nh \le T$. The constant C depends on T, but it is independent of n and h.

The error bound given in this theorem can in principle be deduced by verifying the order conditions (2.7) for exponential general linear methods given in [15]. Here we present a simpler proof based on interpolation errors. Moreover, our proof can easily be generalized to linearized exponential Adams methods, cf. Section 4.2 below.

Proof Let $\widetilde{p}_n$ denote the interpolation polynomial through the exact data

$$\big(t_{n-k+1}, f(t_{n-k+1})\big), \ldots, \big(t_n, f(t_n)\big),$$

where $f(t) = g\big(t, u(t)\big)$. This polynomial has the form

$$\widetilde{p}_n\big(t_n + \theta h\big) = \sum_{j=0}^{k-1} (-1)^j \binom{-\theta}{j} \nabla^j f(t_n),$$

where the backward differences are defined by

$$\nabla^0 f(t_m) = f(t_m), \qquad \nabla^j f(t_m) = \nabla^{j-1} f(t_m) - \nabla^{j-1} f(t_{m-1}), \qquad j = 1, 2, \ldots.$$

Its interpolation error is given by

$$f(t_n + \theta h) - \widetilde{p}_n(t_n + \theta h) = h^k (-1)^k \binom{-\theta}{k} f^{(k)}\big(\zeta(\theta)\big) \tag{4.3}$$

for certain intermediate times $\zeta(\theta) \in [t_{n-k+1}, t_{n+1}]$. The variation-of-constants formula allows us to write the solution of (1.1) in the form

$$u(t_{n+1}) = \mathrm{e}^{-hA} u(t_n) + h \int_0^1 \mathrm{e}^{-h(1-\theta)A} \widetilde{p}_n(t_n + \theta h) \mathrm{d}\theta + \delta_{n+1} \tag{4.4}$$

with defect

$$\delta_{n+1} = h \int_0^1 \mathrm{e}^{-h(1-\theta)A} \big(f(t_n + \theta h) - \widetilde{p}_n(t_n + \theta h) \big) \mathrm{d}\theta.$$

Due to (4.3) and (4.1) this defect is bounded by

$$\|\delta_{n+1}\| \le C h^{k+1} M, \qquad \|\delta_{n+1}\|_V \le C h^{k+1-\alpha} M, \qquad M = \sup_{0 \le t \le t_{n+1}} \|f^{(k)}(t)\|.$$

Let $e_n = u_n - u(t_n)$ denote the error at time t_n with $e_0 = 0$. Taking the difference between (2.4) and (4.4) yields the error recursion

$$e_{n+1} = \mathrm{e}^{-hA} e_n + h \int_0^1 \mathrm{e}^{-h(1-\theta)A} \big(p_n(t_n + \theta h) - \widetilde{p}_n(t_n + \theta h) \big) \mathrm{d}\theta - \delta_{n+1}. \tag{4.5}$$

We solve this recursion to get

$$e_n = h \sum_{j=0}^{n-1} \mathrm{e}^{-(n-j-1)hA} \left(\int_0^1 \mathrm{e}^{-h(1-\theta)A} \big(p_j(t_j + \theta h) - \widetilde{p}_j(t_j + \theta h) \big) \mathrm{d}\theta - \frac{1}{h} \delta_{j+1} \right).$$

We next use the Lipschitz condition (with constant L) from Assumption 4.2 and the stability bound (4.1) to estimate terms of the form

$$\Big\| \mathrm{e}^{-(n-j)hA} \Big(g(t_j, u_j) - g\big(t_j, u(t_j)\big) \Big) \Big\|_V \le C_\gamma L t_{n-j}^{-\alpha} \|e_j\|_V.$$

Note that this bound is uniform as long as the numerical solution remains sufficiently close to the exact solution. This is the case for H sufficiently small as the present proof shows. Since

$$t_j^{-\alpha} \le C t_{j+m}^{-\alpha}, \qquad 0 \le m \le k-1,$$

we have

$$\begin{aligned}
&\left\| \mathrm{e}^{-(n-j)hA} \big(p_j(t_j+\theta h) - \widetilde{p}_j(t_j+\theta h) \big) \right\|_V \\
&\qquad \le C \sum_{\ell=j-k+1}^{j} \left\| \mathrm{e}^{-(n-j)hA} \Big(g(t_\ell, u_\ell) - g\big(t_\ell, u(t_\ell)\big) \Big) \right\|_V \\
&\qquad \le C \sum_{\ell=j-k+1}^{j} t_{n-\ell}^{-\alpha} \, \|e_\ell\|_V \, .
\end{aligned}$$

From this we finally infer the estimate

$$\|e_n\|_V \le C \max_{j=1,\dots,k-1} \|e_j\|_V + Ch \sum_{j=0}^{n-1} \frac{1}{t_{n-j}^{\alpha}} \Big(\|e_j\|_V + h^k \Big) + C \|\delta_n\|_V \, .$$

The stated error bound then follows from a discrete Gronwall lemma (Lemma 2.15 in [11]). □

Remark 4.4 (a) The above proof shows that exponential Adams methods converge with full order for linear problems

$$u'(t) + Au(t) = f(t), \qquad u_0 = u(0),$$

if the right-hand side f is sufficiently smooth. In contrast to standard integrators, *no* compatibility conditions at $t = 0$ are required for abstract parabolic problems.

(b) Under the assumptions of the theorem, the starting procedure (2.8) yields starting values $(u_1, \dots, u_{k-1})$ which satisfy (4.2).

(c) For $\alpha = 0$, Assumption 4.1 can obviously be relaxed to the requirement that $(-A)$ is the infinitesimal generator of a strongly continuous semigroup e^{-tA} on X.

We illustrate our convergence result with a numerical example. Consider the semilinear parabolic problem

$$\frac{\partial U}{\partial t}(x,t) - \frac{\partial^2 U}{\partial x^2}(x,t) = \frac{1}{1+U(x,t)^2} + \Phi(x,t) \tag{4.6}$$

with $x \in [0,1]$ and $t \in [0,1]$, subject to homogeneous Dirichlet boundary conditions. The source function Φ is chosen in such a way that the exact solution of the problem is $U(x,t) = x(1-x)\,\mathrm{e}^t$. Discretizing (4.6) in space by standard finite differences with 200 grid points yields a stiff initial value problem of the form (1.2). We integrate this system in time with exponential k-step Adams methods for $k = 1, \dots, 6$ and compute the errors in a discrete L^2 norm. The results which are displayed in Fig. 4.1 in a double-logarithmic diagram are in perfect agreement with Theorem 4.3.

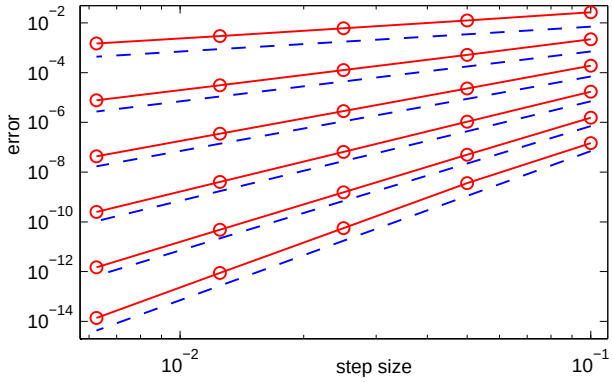

Fig. 4.1 Order plot for the exponential k-step Adams methods ($k = 1,\dots,6$) applied to example (4.6). The problem is discretized in space with 200 grid points and integrated in time with constant step sizes. The dashed lines are straight lines of slope k. They are added for purpose of comparison

4.2 Convergence of linearized exponential multistep methods

For simplicity, we restrict our error analysis to semilinear problems fulfilling (2.1). In this case, (3.1) takes the form

$$\begin{aligned} J_n &= -A + \frac{\partial g}{\partial u}(t_n,u_n), \qquad d_n = \frac{\partial g}{\partial t}(t_n,u_n), \\ g_n(t,u) &= g(t,u) - \frac{\partial g}{\partial u}(t_n,u_n)u - d_n t. \end{aligned} \tag{4.7}$$

Our main hypothesis on the nonlinearity g is the following.

Assumption 4.5 *We assume that the initial value problem* (1.2) *possesses a sufficiently smooth solution $u : [0,T] \to V$ with derivatives in V, and that $g : [0,T] \times V \to X$ is Fréchet-differentiable in a strip along the exact solution. All occurring derivatives are assumed to be uniformly bounded.* ○

We are now in the position to prove our convergence theorem.

Theorem 4.6 *Let the initial value problem* (1.2) *satisfy Assumptions* 4.1 *and* 4.5*, and consider for its numerical solution the k-step linearized exponential Adams method* (3.7) *with step size h satisfying $0 < h \le H$ for H sufficiently small. Let $f(t) = g\big(t,u(t)\big)$ and assume that $f \in C^{k+1}([0,T],X)$. Then, for*

$$\big\|u_j - u(t_j)\big\|_V \le c_0 h^{k+1}, \qquad j = 1,\dots,k-1, \tag{4.8}$$

the error bound

$$\|u_n - u(t_n)\|_V \le C \cdot h^{k+1} \sup_{0\le t\le t_n} \Big(\|f^{(k+1)}(t)\| + \|u^{(k+1)}(t)\|_V \Big)$$

holds uniformly in $0 \le nh \le T$. The constant C depends on T, but it is independent of n and h.

Proof The proof of this theorem is very close to that of Theorem 4.3. This time, we consider the Hermite interpolation polynomial $\widetilde{p}_n$ through the exact data

$$\big(t_{n-k+1}, f_n(t_{n-k+1})\big), \dots, \big(t_n, f_n(t_n)\big),$$

satisfying $\widetilde{p}_n'(t_n) = f_n'(t_n)$. Here we denoted $f_n(t) = g_n\big(t, u(t)\big)$. This interpolation polynomial is given by

$$\widetilde{p}_n\big(t_n+\theta h\big) = f_n\big(t_n\big) + \theta h f_n'(t_n) + \sum_{j=1}^{k-1} (-1)^j \theta \binom{-\theta}{j} \left(h f_n'(t_n) - \sum_{\ell=1}^{j} \tfrac{1}{\ell} \nabla^\ell f_n(t_n) \right).$$

The backward differences are defined by

$$\nabla^0 f_n(t_m) = f_n(t_m), \qquad \nabla^j f_n(t_m) = \nabla^{j-1} f_n(t_m) - \nabla^{j-1} f_n(t_{m-1}), \qquad j = 1,2,\dots.$$

Its interpolation error is given by

$$f_n(t_n+\theta h) - \widetilde{p}_n(t_n+\theta h) = h^{k+1} (-1)^k \theta \binom{-\theta}{k} \frac{f_n^{(k+1)}\big(\zeta(\theta)\big)}{k+1}$$

for certain intermediate times $\zeta(\theta) \in [t_{n-k+1}, t_{n+1}]$. The variation-of-constants formula (3.3) allows us then to write the solution of (1.1) as

$$u(t_{n+1}) = \mathrm{e}^{hJ_n} u(t_n) + h \int_0^1 \mathrm{e}^{h(1-\theta)J_n} \big((t_n+\theta h) d_n + \widetilde{p}_n(t_n+\theta h) \big) + \delta_{n+1} \tag{4.9}$$

with defect

$$\delta_{n+1} = h \int_0^1 \mathrm{e}^{h(1-\theta)J_n} \big(f_n(t_n+\theta h) - \widetilde{p}_n(t_n+\theta h) \big) \mathrm{d}\theta.$$

Due to (4.1) and the smoothness of f_n, the defect is bounded by

$$\|\delta_{n+1}\| \le C h^{k+2} M, \qquad \|\delta_{n+1}\|_V \le C h^{k+2-\alpha} M,$$
$$M = \sup_{0\le t\le t_{n+1}} \Big(\|f^{(k+1)}(t)\| + C \|u^{(k+1)}(t)\|_V \Big).$$

Taking the difference between (3.7a) and (4.9) yields the error recursion

$$e_{n+1} = \mathrm{e}^{hJ_n} e_n + h \int_0^1 \mathrm{e}^{h(1-\theta)J_n} \big(\widehat{p}_n(t_n+\theta h) - \widetilde{p}_n(t_n+\theta h) \big) \mathrm{d}\theta - \delta_{n+1}.$$

We solve this error recursion and use the differentiability of g (cf. Assumption 4.5) to bound the difference of the interpolation polynomials in a similar way as in the proof of the previous theorem. In particular, applying the stability result of [12, Appendix A] (which might introduce an additional step size restriction) yields

$$\Big\| \mathrm{e}^{hJ_{n-1}} \cdots \mathrm{e}^{hJ_{j+1}} \Big(g_j\big(t_j, u(t_j)\big) - g_j(t_j, u_j) \Big) \Big\|_V \le C t_{n-j}^{-\alpha} \|e_j\|_V.$$

In order to bound the additional term

$$f_n'(t_n) = \frac{\partial g_n}{\partial t}\big(t_n, u(t_n)\big) + \frac{\partial g_n}{\partial u}\big(t_n, u(t_n)\big) u'(t_n),$$

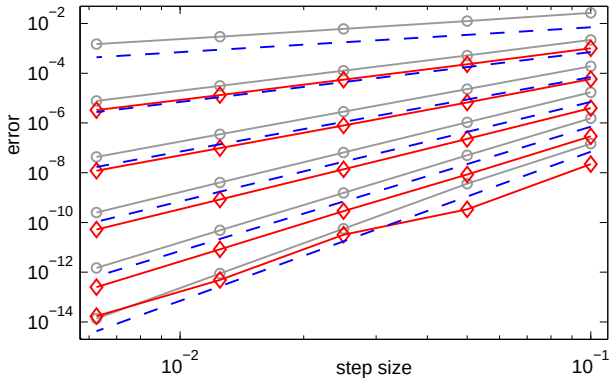

Fig. 4.2 Order plot for the linearized exponential k-step Adams methods (diamonds, $k = 1,\ldots,5$) applied to example (4.6). The problem is discretized in space with 200 grid points and integrated in time with constant step sizes. The results obtained with the exponential k-step Adams methods (circles) for $k = 1,\ldots,6$ are drawn for comparison. The dashed lines are straight lines of slope k. They are added for purpose of comparison

we make use of the relations (3.4). Note that the numerical solution remains sufficiently close to the exact solution for H sufficiently small. This guarantees the uniform boundedness of the arising Lipschitz constants. Employing all these bounds finally shows that

$$\|e_n\|_V \leq C \max_{j=1,\ldots,k-1} \|e_j\|_V + Ch \sum_{j=0}^{n-1} \frac{1}{t_{n-j}^{\alpha}} \left(\|e_j\|_V + h^{k+1} \right) + C \|\delta_n\|_V .$$

The application of a discrete Gronwall lemma (Lemma 2.15 in [11]) thus concludes the proof. □

Remark 4.7 Under the assumptions of the theorem, the starting values computed from (3.10) satisfy (4.8).

In order to illustrate the convergence result of Theorem 4.6, we take up example (4.6) and integrate it this time with the linearized exponential k-step Adams methods for $k = 1,\ldots,5$. The results, together with the results of the previous experiment are displayed in Fig. 4.2. The linearized methods obviously have smaller error constants.

5 Implementation issues

In this section, we comment on possible implementations of the matrix functions arising in (linearized) exponential multistep methods. Further issues like variable step sizes and variable order implementations will be discussed elsewhere.

5.1 Diagonalization

If the dimension of the problem is small enough or if the diagonalization of the matrix A can be computed efficiently (by fast Fourier transformation, e.g.), then the initial value problem (1.2) should be transformed into the basis of eigenvectors. The matrix functions can be precomputed on the eigenvalues of A and used for all time steps. Clearly, for an implementation using diagonalization, exponential Adams methods are much more attractive than linearized multistep methods, since the latter require a new diagonalization of J_n in each time step.

5.2 (Rational) Krylov subspace methods

For large scale problems, (rational) Krylov subspace methods can be applied to approximate the products of matrix functions with vectors. Since this approximation does not reuse computations from previous time steps, it does not matter that the matrix J_n is different in each of the time steps (except that the evaluation of J_n itself might be expensive). Since Krylov subspace methods benefit from properties of the vector which multiplies the matrix function, one should exploit that the backward differences used in (3.7a) satisfy $\nabla G_{n,n} = O(h^2)$ due to (3.4) and $\nabla^\ell G_{n,n} = O(h^\ell)$, $\ell \geq 2$ if the assumptions of Theorem 4.6 are satisfied. We thus rewrite the scheme (3.7) as

$$u_{n+1} = u_n + h\varphi_1(hJ_n)F(t_n,u_n) + h^2\varphi_2(hJ_n)d_n + h\sum_{\ell=1}^{k-1}\beta_{k,\ell}(hJ_n)\nabla^\ell G_{n,n}, \tag{5.1a}$$

where

$$\beta_{k,\ell} = \tfrac{1}{\ell}\sum_{j=\ell}^{k-1}\widehat{\gamma}_{j+1}. \tag{5.1b}$$

Table 5.1 shows these coefficients in terms of φ-functions.

For purpose of illustration, we consider the following two-dimensional parabolic problem

$$\frac{\partial U}{\partial t}(x_1,x_2,t) - \Delta U(x_1,x_2,t) = \frac{1}{1+U(x_1,x_2,t)^2} \tag{5.2}$$

with $(x_1,x_2) \in [0,1]^2$ and $t \in [0,0.2]$, subject to homogenous Dirichlet boundary conditions. We discretized (5.2) by standard finite differences with $N = 75$ grid points in each direction and integrated the resulting semidiscrete problem with the linearized exponential 5-step method using Krylov subspace methods. The left picture of Fig. 5.1 shows the norms of the backward differences $\nabla^m G_{n,n}$, $m = 1,\dots,4$. For this example, the first differences are even smaller than the second differences. The different behavior of the differences within the first time steps is due to the fact that the initial data does not satisfy the compatibility conditions at $t = 0$.

The right picture of Fig. 5.1 shows the number of Krylov steps required to achieve the desired accuracy of $O(h^{k+2})$. As expected, most of the Krylov steps are required to approximate $\varphi_1(hJ_n)F(t_n,u_n)$, while the products of the coefficients with the backward differences can be approximated in low dimensional Krylov subspaces.

k	m	$\beta_{k,\ell}$
2	1	$-2\varphi_3$
3	1	$-3\varphi_4-3\varphi_3$
	2	$-\frac{3}{2}\varphi_4-\frac{1}{2}\varphi_3$
4	1	$-4\varphi_5-6\varphi_4-\frac{11}{3}\varphi_3$
	2	$-2\varphi_5-3\varphi_4-\frac{5}{6}\varphi_3$
	3	$-\frac{4}{3}\varphi_5-\varphi_4-\frac{2}{9}\varphi_3$
5	1	$-5\varphi_6-10\varphi_5-\frac{35}{4}\varphi_4-\frac{25}{6}\varphi_3$
	2	$-\frac{5}{2}\varphi_6-5\varphi_5-\frac{35}{8}\varphi_4-\frac{13}{12}\varphi_3$
	3	$-\frac{5}{3}\varphi_6-\frac{10}{3}\varphi_5-\frac{23}{12}\varphi_4-\frac{7}{18}\varphi_3$
	4	$-\frac{5}{4}\varphi_6-\frac{3}{2}\varphi_5-\frac{11}{16}\varphi_4-\frac{1}{8}\varphi_3$

Table 5.1 The coefficients $\beta_{k,\ell}$ of method (5.1)

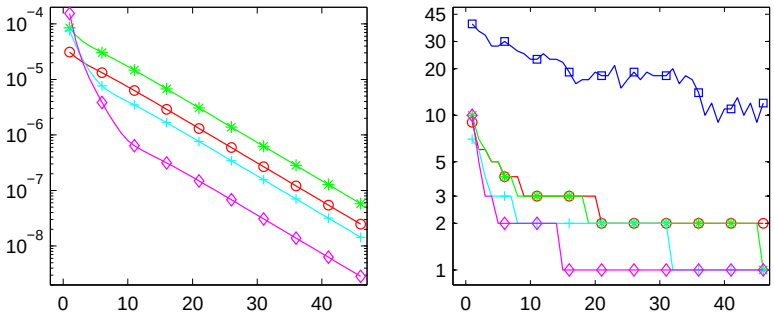

Fig. 5.1 Norms of backward differences and employed Krylov dimensions. The curves represent function values (squares), first differences (circles), second differences (stars), third differences (pluses), fourth differences (diamonds)

Analogously, we rewrite the starting procedure (3.10) by defining

$$\widehat{\beta}_{k,m,\ell}(z)=\frac{(-1)^\ell}{\ell}\sum_{j=\ell}^{k-1}\widehat{\sigma}_{m,j}(z).$$

This yields the nonlinear system of equations

$$u_m=u_0+(mh)\varphi_1(mhJ_0)F(t_0,u_0)+(mh)^2\varphi_2(mhJ_0)d_0+h\sum_{\ell=1}^{k-1}\widehat{\beta}_{k,m,\ell}(hJ_0)\Delta^\ell G_{0,0},$$

which can be solved by fixed point iteration if h is sufficiently small.

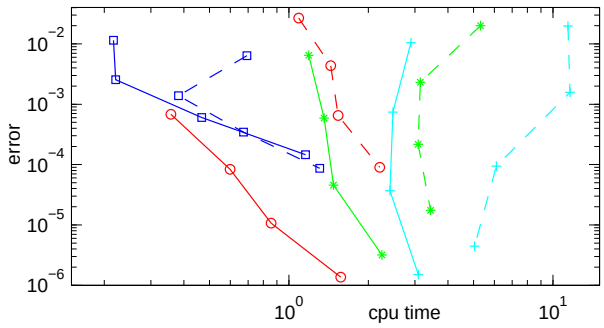

Fig. 5.2 Error versus cpu time for the exponential $(k+1)$-step Adams methods (dashed lines) and the linearized exponential k-step Adams methods (lines) for the Brusselator problem from [10, Section 7.1] with $\alpha = 0.02$. The cases $k = 1$ (squares), $k = 2$ (circles), $k = 3$ (stars) and $k = 4$ (pluses) are shown

To illustrate the efficiency of the linearized exponential Adams methods for particular examples, we consider the Brusselator problem from Section 7.1 in [10] with $\alpha = 0.02$. In our experiment, the products of the matrix functions with vectors are approximated by the Arnoldi method. Figure 5.2 shows the error of different methods as a function of the cpu time. As expected, the linearized exponential methods clearly outperform the exponential Adams methods in this example. The reasons for this behavior are that the evaluation of the Jacobian is relatively cheap and that the vectors multiplying the matrix functions have smaller norm, which results in smaller Krylov subspaces. Moreover, the linearized methods have smaller error constants.

5.3 Multiple time stepping

The construction of exponential Adams methods was based on replacing the nonlinearity g in the variation-of-constants formula (2.2) by the local interpolation polynomial p_n defined in (2.3). Thus the method can also be interpreted as solving the differential equation

$$y_n'(\tau) = -Ay_n(\tau) + p_n(t_n+\tau), \qquad y_n(0) = u_n, \tag{5.3}$$

on the time interval $[0,h]$ exactly and setting $u_{n+1} = y_n(h)$. For an approximation one could also solve (5.3) by an explicit scheme using smaller time steps. The method can then be interpreted as a multiple time stepping procedure using a macro time step h for sampling the nonlinearity g and a micro time step for the solution of (5.3). Since the method requires only one evaluation of g per macro time step, such a multiple time stepping implementation is attractive if the evaluation of the nonlinearity g is much more expensive than a few matrix vector multiplications with A.

For the linearized exponential multistep methods we have $u_{n+1} = \widehat{y}_n(h)$, where $\widehat{y}_n(h)$ is the exact solution of

$$\widehat{y}_n'(\tau) = J_n\widehat{y}_n(\tau) + (t_n+\tau)d_n + \widehat{p}_n(t_n+\tau), \qquad \widehat{y}_n(0) = u_n, \tag{5.4}$$

over the interval $[0,h]$. The polynomial $\widehat{p}_n$ was defined in (3.5). Hence a multiple time stepping implementation is possible for these methods as well.

6 Application to partitioned problems

As a further application of exponential multistep methods, we consider problems where the stiff and the nonstiff components can be distinguished:

$$\begin{bmatrix} v \\ w \end{bmatrix}' = \begin{bmatrix} L & Z \\ Y & B \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} + \begin{bmatrix} a(t,v,w) \\ b(t,v,w) \end{bmatrix} =: J \begin{bmatrix} v \\ w \end{bmatrix} + \begin{bmatrix} a(t,v,w) \\ b(t,v,w) \end{bmatrix}. \tag{6.1}$$

Here, the stiff components are denoted by v and the nonstiff components by w, respectively. Let

$$P = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}$$

be the projector onto the stiff components. In this situation we can apply an exponential Adams method (2.5) with

$$-A = JP = \begin{bmatrix} L & 0 \\ Y & 0 \end{bmatrix}, \qquad g(t,v,w) = \begin{bmatrix} 0 & Z \\ 0 & B \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} + \begin{bmatrix} a(t,v,w) \\ b(t,v,w) \end{bmatrix}. \tag{6.2}$$

For an error analysis of exponential Adams methods applied to this partitioning, we have to verify the assumptions of Theorem 4.3. For this purpose, we assume that the spectrum of L is bounded away from the origin, that L fulfills Assumption 4.1 on a Banach space X_L, and that B is a bounded operator on a Banach space X_B. We then consider the Banach spaces $X = X_L \times X_B$ and $V = V_L \times X_B$, where

$$V_L = \{v \in X_L \mid L^\alpha v \in X_L\} \subset X_L.$$

Assumption 4.1 is obviously fulfilled for the operator A defined in (6.2), if $YL^{-1} : X_L \to X_B$ is bounded. Assumption 4.2 is fulfilled, if $Z : X_B \to X_L$ is bounded and if $a : [0,T] \times V_L \times X_B \to X_L$ and $b : [0,T] \times V_L \times X_B \to X_B$ are locally Lipschitz continuous in a strip along the exact solution.

For an analytic function ϕ it is easily verified that

$$\phi(-hA) = \begin{bmatrix} \phi(hL) & 0 \\ hY\phi^{[1]}(hL) & \phi(0)I \end{bmatrix}, \tag{6.3}$$

where

$$\phi^{[1]}(z) = \frac{\phi(z) - \phi(0)}{z}. \tag{6.4}$$

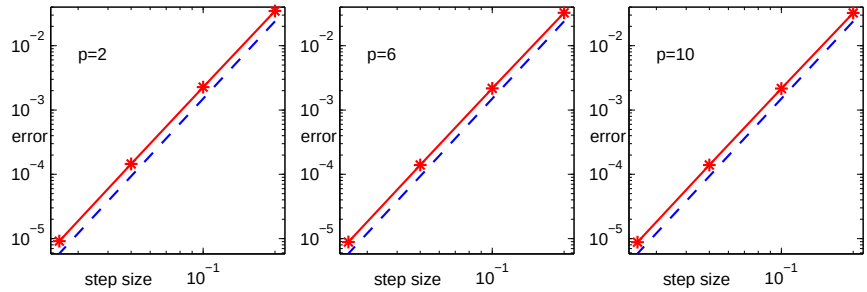

Fig. 6.1 Order plots for different refinement factors p. The results were obtained with the exponential 4-step Adams method applied to (6.6) and clearly show order four (which is the slope of the dashed line)

The block structure of A can thus be exploited in the implementation. Using (6.3), the exponential Adams method (2.5a), applied to (6.1), (6.2) reads

$$\begin{aligned} v_{n+1} &= v_n + h\varphi_1(hL)\big(Lv_n + Zw_n + a_n\big) + h\sum_{j=1}^{k-1}\gamma_j(hL)\nabla^j\big(Zw_n + a_n\big), \\ w_{n+1} &= w_n + hY\left(\varphi_1(hL)v_n + h\varphi_2(hL)(Zw_n + a_n) + h\sum_{j=1}^{k-1}\gamma_j^{[1]}(hL)\nabla^j(Zw_n + a_n)\right) \\ &\quad + h\sum_{j=0}^{k-1}\gamma_j(0)\nabla^j(Bw_n + b_n). \end{aligned}$$

Alternatively, if in addition to the assumptions posed above, the operator $Y : X_L \to X_B$ is bounded, then Assumption 4.1 and 4.2 are fulfilled for

$$-A = \begin{bmatrix} L & 0 \\ 0 & 0 \end{bmatrix}, \qquad g(t,v,w) = \begin{bmatrix} 0 & Z \\ Y & B \end{bmatrix}\begin{bmatrix} v \\ w \end{bmatrix} + \begin{bmatrix} a(t,v,w) \\ b(t,v,w) \end{bmatrix}. \tag{6.5}$$

In this case, the exponential Adams method reads

$$\begin{aligned} v_{n+1} &= v_n + h\varphi_1(hL)\big(Lv_n + Zw_n + a_n\big) + h\sum_{j=1}^{k-1}\gamma_j(hL)\nabla^j\big(Zw_n + a_n\big), \\ w_{n+1} &= w_n + h\sum_{j=0}^{k-1}\gamma_j(0)\nabla^j(Yv_n + Bw_n + b_n). \end{aligned}$$

Note that the update of the stiff components is the same as before. However, the nonstiff components can be computed more efficiently since no matrix functions are required.

As an application we consider a discretization of the damped wave equation

$$\frac{\partial^2 U}{\partial t^2}(x,t) + \sigma\frac{\partial U}{\partial t}(x,t) = \frac{\partial^2 U}{\partial x^2}U(x,t) \tag{6.6}$$

which was also presented in [5]. We equip this problem with homogeneous Dirichlet boundary conditions on the interval $[0,6]$. Its exact solution is

$$U(x,t) = \frac{2\mathrm{e}^{-\frac{\sigma t}{2}}}{\sqrt{4\pi^2-\sigma^2}} \sin(\pi x) \sin\left(\frac{t}{2}\sqrt{4\pi^2-\sigma^2}\right). \tag{6.7}$$

We discretized (6.6) with fourth-order finite differences in space and locally refined the grid in the subinterval $[2,4]$, where we reduced the grid size by a factor of $p = 2,6,10$, respectively. Fig. 6.1 shows the errors of the exponential 4-step Adams method with $h = \Delta x_c/6$ for coarse grid sizes $\Delta x_c = 0.2, 0.1, 0.05, 0.025$ which are used in $[0,2) \cup (4,6]$. The matrix A was chosen as in (6.2) with the blocks L, Y corresponding to the refined grid points and $a = b = 0$. For this example, it turns out that even the exponential 3-step Adams method is accurate enough to give fourth-order convergence in the coarse grid size. We omit the graphs since the curves cannot be distinguished from those of the 4-step method.

As an alternative that avoids matrix functions, the resulting fine-grid equations can also be solved by an explicit time stepping scheme. Such an approach requires small time steps on the time interval $[t_n, t_{n+1}]$ and leads to a multiple time stepping method as described in Section 5.3. For the considered problem, it gives the explicit local-time stepping method proposed in [5]. For related methods and ideas, we refer to [6, 7].

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