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Convergence of rational multistep methods of Adams-Padé type

Winfried Auzinger · **Magdalena Łapińska**

Dedicated to the memory of Jan Verwer (1946–2011)

Abstract Rational generalizations of multistep schemes, where the linear stiff part of a given problem is treated by an A-stable rational approximation, have been proposed by several authors, but a reasonable convergence analysis for stiff problems has not been provided so far. In this paper we directly relate this approach to exponential multistep methods, a subclass of the increasingly popular class of exponential integrators. This natural, but new interpretation of rational multistep methods enables us to prove a convergence result of the same quality as for the exponential version. In particular, we consider schemes of rational Adams type based on A-acceptable Padé approximations to the matrix exponential. A numerical example is also provided.

Keywords rational multistep schemes · stiff initial value problems · evolution equations · Adams schemes · Padé approximation · convergence

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

1 Introduction

The generalization of classical multistep methods, in particular Adams methods, to make them applicable to stiff initial value problems, has been considered by several authors, see [2,13,17,20,19]. The basic idea is to incorporate an A-stable rational approximation $R(hA)$ to e^{hA}, where h is the step size and A is the matrix representing the leading stiff part of the problem. This approach leads to rational versions of

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multistep schemes, of semi-implicit type. In particular we refer to the work of Verwer [20], where such a construction is explicated and shown to be well-defined under appropriate consistency requirements. The coefficients of the method are obtained by solving certain Vandermonde systems derived from the consistency conditions.

By construction, such a scheme has a given classical local order and it is A-stable. However, this does not answer the question how the global error actually behaves in general. In the integration of stiff systems, there is the well-known effect of order reduction which may drastically reduce the accuracy of the scheme even for simple semilinear stiff problems. In all these earlier papers, numerical examples are given and the error behavior with increasing stiffness is studied. What has been missing is a stiff convergence theory, i.e., a priori global error bounds of the form $C h^p$ with error constants independent on the stiffness.

In the meantime, various types of exponential integrators have been extensively studied in the literature. In particular, exponential Adams methods have been considered in detail, cf., e.g., [3,4,10,11,15], and convergence results are available for this class of methods, cf. [10,11].

The main purpose of this paper is to develop a convergence theory for rational multistep methods. In particular, we show how rational Adams methods can be derived in a natural way by rational modification of exponential Adams methods. This leads to a simple explicit recursion for the coefficients, and the convergence properties can be studied along the lines of the exponential approach. However, the derivation of rigorous error bounds is not straightforward. It requires an appropriate reformulation of the scheme, and uniform approximation estimates for the underlying rational approximations $R(hA)$ to e^{hA}. We prove a convergence theorem for Adams-Padé methods, where $R(hA)$ is chosen as an A-stable Padé approximation to e^{hA}; see Theorem 4.1 below.

We consider an initial value problem for a function $u\colon [0,T] \to \mathbb{C}^d$,

$$u'(t) = F(t,u(t)), \qquad u(0) = u_0. \tag{1.1}$$

In particular, semilinear problems of the form

$$u'(t) = A\,u(t) + g(t,u(t)), \qquad u(0) = u_0, \tag{1.2}$$

will be analyzed, with $A \in \mathbb{C}^{d\times d}$ a constant matrix. The exact solution of (1.2) is denoted by $u(t)$. By $\|\cdot\|$ we denote the Euclidean norm on $\mathbb{C}^d$ as well as its associated matrix norm. Throughout, C denotes a generic constant independent of the problem data.

Assumption 1.1

(a) $A \in \mathbb{C}^{d\times d}$ is a dissipative matrix, i.e., $\operatorname{Re} A = \frac{1}{2}(A + A^*)$ is negative semidefinite. This implies $\|\mathrm{e}^{tA}\| \le 1$ for all $t > 0$.

(b) The function $g\colon [0,T]\times\mathbb{C}^d \to \mathbb{C}^d$ is locally Lipschitz continuous in a neighborhood of the exact solution $u(t)$.

All error bounds discussed in the sequel are naturally influenced by a Lipschitz bound for g. Thus, a reasonable error behavior is to be expected for problems where the nonlinear part is smooth or only mildly stiff, which is a natural consequence of any semi-implicit approach for the numerical solution.

Throughout we use the denotation

$$Z = hA \tag{1.3}$$

where h is the step size used in the numerical integration process.

The paper is organized as follows: in Sect. 2 we give a short review of exponential integrators of Adams type. In Sect. 3 we define a class of rational integrators of Adams type by modifying the recursion defining the coefficients of the exponential version. We collect some basic facts and relate this to prior approaches. Sect. 4 is devoted to the convergence theory of a special class, namely Adams-Padé methods applied to semilinear initial value problems (1.2). This section also contains a reformulation of the schemes beneficial for the convergence analysis, and results concerning the error of Padé approximations to the matrix exponential. In Sect. 5 we present a numerical example and briefly discuss implementation issues and possible generalizations.

Remark 1.1

- Similarly as in [11] for exponential Adams methods, we develop a convergence theory for constant step size h. Here we are not aiming at formulating results in a very general setting, but we stick to the practically relevant finite-dimensional case and formulate our results under the standard assumption 1.1.
- We show that the rational Padé version of a multistep integrator shows the same convergence behavior as the exponential version, which is a nontrivial result already under standard assumptions about the problem at hand. Naturally, the extension of these techniques to more general problem classes will be a relevant topic for further investigations.
- All schemes considered can also be implemented with variable step size, and such approaches have been suggested in the literature (without precise error analysis). Stability problems are not to be expected in this case, because the stiff part of the problem is treated in a one-step fashion. The convergence theory, however, will become technically more involved.
- For a general problem (1.1), 'linearized' methods have also been proposed where, at each grid point t_n, the differential equation is linearized about the current approximation (t_n, u_n):
$$u'(t) = J_n\, u(t) + g_n(t, u(t)), \tag{1.4}$$
with $J_n = F_u(t_n, u_n)$ which plays the role of A in the subsequent integration step. For this linearized version, the stability analysis may become significantly more involved, depending on the assumptions on the problem, see [11].
- Naturally, all these extensions and generalizations are of interest also in the context of rational integrators considered here.
- Some brief remarks concerning implementation issues and a comparison of the rational with the exponential version are given in Sect. 5.

2 Exponential multistep methods of Adams type

According to [4, 10, 11], exponential p-step methods of Adams type are defined in the following way: On an equidistant grid $\{t_n = nh, n = 1, 2, \ldots\}$, approximations $u_n \approx u(t_n)$ are designed by approximating the integral in the variation-of-constants identity

$$u(t_{n+1}) = \mathrm{e}^{hA} u(t_n) + \int_0^h \mathrm{e}^{(h-\tau)A}\, g(t_n+\tau, u(t_n+\tau))\,\mathrm{d}t,$$

by replacing $g(t, u(t))$ with $G_n(t)$, where

$$G_n(t) = \text{Lagrange interpolant of degree } p-1 \text{ at } (t_{n-k}, g_{n-k}),\ k = 0\ldots p-1.$$

Here, $g_{n-k} = g(t_{n-k}, u_{n-k})$ denotes the values available from prior steps. With $Z = hA$, and using a Newton representation for $G_n(t)$, this leads to a p-step recursion of the form [1]

$$u_{n+1} = \mathrm{e}^Z u_n + h \sum_{k=0}^{p-1} \gamma_k(Z)(\nabla^k G_n)_n, \tag{2.1}$$

where $(\nabla^k f)_n$ denotes the k-th backward difference of $f(t)$ over $t_n, \ldots, t_{n-k}$, defined in the usual recursive way. The coefficient matrices $\gamma_k(Z)$ are determined from

$$\gamma_k(z) = (-1)^k \int_0^1 \mathrm{e}^{(1-\theta)z} \binom{-\theta}{k} \mathrm{d}\theta, \quad k \geq 0. \tag{2.2}$$

In [4], the generating function

$$\sum_{k\geq 0} \gamma_k(z)\zeta^k = \frac{(1-\zeta)\mathrm{e}^z - 1}{(1-\zeta)(z + \log(1-\zeta))} =: \Gamma(\zeta; z) \tag{2.3}$$

is used to derive the following recursion for the $\gamma_k(z)$:

$$\gamma_0(z) = z^{-1}(\mathrm{e}^z - 1), \tag{2.4}$$

and

$$\gamma_k(z) = z^{-1}\Big(\sum_{j=0}^{k-1} \frac{\gamma_j(z)}{k-j} \ - 1\Big), \quad k \geq 1. \tag{2.5}$$

Here, $\gamma_0(z) = \varphi_1(z)$, the first '$\varphi$-function', and the $\gamma_k(z)$ can also be expressed as linear combinations of the higher φ_j-functions. See [10] for the recursive definition of the $\varphi_j(z)$, and [11] for representation of the $\gamma_k(z)$ in terms of the $\varphi_j(z)$. In [14], an explicit representation of the $\gamma_k(z)$ in terms of Stirling numbers is given.

Remark 2.1 This exponential scheme (as well as our rational modification introduced in Sect. 3) can be considered as a generalization of the classical Adams-Bashforth schemes for $u'(t) = g(t, u(t))$ (corresponding to $A = 0$), and (2.5) is a generalization of an analogous recursion for the Adams schemes given in [8, Chap. 5] (see also [6,

[1] Throughout we are assuming that $p \geq 2$. For related approaches see [1, 3].

Chap. III]).

Fully nonlinear-implicit versions (analogous to Adams-Moulton schemes, see [8]) or predictor-corrector implementations suggest themselves for the case where the nonlinearity $g(t,u(t))$ also shows a stiff behavior. Such versions are not further considered in the present paper.

The following convergence theorem is an immediate consequence of [11, Theorem 4.3] (see also [10, Theorem 2.27]). Naturally, it is assumed that p sufficiently accurate initial values $u_0,\ldots,u_{p-1}$ have been provided for starting the integrator.

Theorem 2.1 *Let the initial value problem (1.2) satisfy Assumption 1.1, and consider for its numerical solution the p-step exponential Adams method (2.1) with step size h satisfying* $0<h<H$ *with H sufficiently small. Let* $f(t)=g(t,u(t))$ *and assume that* $f\in C^p([0,T],\mathbb{C}^d)$*. Then, for*

$$\|u_n-u(t_n)\|\le c_0\,h^p,\quad n=0\ldots p-1,$$

the error bound

$$\|u_n-u(t_n)\|\le C\,c_0\,h^p+C\,h^p\sup_{0\le t\le t_n}\|f^{(p)}(t)\|$$

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

For efficient implementation, (2.1) is usually reformulated as a corrected exponential Euler step, see [10].

3 Rational multistep methods of Adams type

We now introduce a class of rational Adams methods, replacing $\mathrm{e}^Z=\mathrm{e}^{hA}$ by a rational approximation $R(Z)$, with

$$R(z)=\frac{P(z)}{Q(z)},\quad P(0)=Q(0)=1. \tag{3.1}$$

This will of course be chosen to be sufficiently consistent to e^z and A-acceptable.

3.1 Definition of rational Adams methods

The basic structure of our rational scheme is the same as for exponential Adams methods. The approximations for $u(t_n)$ are denoted by $\tilde{u}_n$, and we define them via a recursion analogous to (2.1),

$$\tilde{u}_{n+1}=R(Z)\tilde{u}_n+h\sum_{k=0}^{p-1}\tilde{\gamma}_k(Z)(\nabla^k\tilde{G}_n)_n, \tag{3.2}$$

where $\tilde{G}_n(t)$ interpolates the $(t_{n-p+j}, \tilde{g}_{n-t+j}) = (t_{n-p+j}, g(t_{n-t+j}, \tilde{u}_{n-p+j}))$. The modified coefficient matrices $\tilde{\gamma}(Z)$ are rational versions of the $\gamma_k(Z)$ defined analogously to (2.4),(2.5),

$$\tilde{\gamma}_0(z) = z^{-1}(R(z) - 1), \tag{3.3}$$

and

$$\tilde{\gamma}_k(z) = z^{-1}\Big(\sum_{j=0}^{k-1} \frac{\tilde{\gamma}_j(z)}{k-j} \; - 1\Big), \quad k \geq 1. \tag{3.4}$$

As a particular choice, we will consider $R(z)$ to be a subdiagonal Padé approximation to e^z. For the moment we only assume:

Assumption 3.1

$R(z)$ is well-defined for $\operatorname{Re} z \leq 0$,

$R(z)$ is consistent of order $q \geq p-1$: $\quad R(z) - \mathrm{e}^z = \mathscr{O}(|z|^{q+1})$ for $z \to 0$.

Remark 3.1 Since the $\gamma_k(z)$ are linear combinations of (exponential) φ_j-functions, it is clear by construction that the $\tilde{\gamma}_k(z)$ are analogous linear combinations of the corresponding 'rational $\tilde{\varphi}_j$-functions', again satisfying an analogous recursion with $R(z)$ instead of e^z. However, if $R(z)$ is a Padé approximation of e^z, the $\tilde{\varphi}_j(z)$, $\tilde{\gamma}_k(z)$ will not be Padé approximations of the $\varphi_j(z)$, $\gamma_k(z)$. Rather, under Assumption 3.1 we obtain successively lower order approximations with a common denominator polynomial, see Lemma 3.1. For the Padé choice see Corollary 4.3 below, and this exactly satisfies our needs.

3.2 Basic properties

The $\gamma_k(z)$ from (2.2) are entire functions. Under the appropriate consistency condition on $R(z)$, the $\tilde{\gamma}_k(z)$ are also well-defined and satisfy the following elementary properties.

Lemma 3.1 *Under Assumption 3.1, the $\tilde{\gamma}_k(z), k = 0 \ldots p-1$, are well-defined for* $\operatorname{Re} z \leq 0$. *They can be written as*

$$\tilde{\gamma}_k(z) = \frac{\tilde{P}_k(z)}{z^{k+1} Q(z)}, \tag{3.5}$$

with certain polynomials $\tilde{P}_k(z)$, and $Q(z)$ from (3.1). The $\tilde{\gamma}_k(z)$ are consistent approximations to the $\gamma_k(z)$,

$$\tilde{\gamma}_k(z) = \gamma_k(z) + \mathscr{O}(|z|^{q-k}) \;\; \textit{for} \;\; z \to 0, \quad k = 0 \ldots p-1. \tag{3.6}$$

Proof For $k = 0$ we have

$$\tilde{\gamma}_0(z) = \frac{P(z) - Q(z)}{z\,Q(z)} =: \frac{\tilde{P}_0(z)}{z\,Q(z)}, \qquad \tilde{\gamma}_0(z) - \gamma_0(z) = \frac{R(z) - \mathrm{e}^z}{z} = \mathscr{O}(|z|^q).$$

For $k > 0$ we inductively assume

$$\tilde{\gamma}_j(z) = \frac{\tilde{P}_j(z)}{z^{j+1}Q(z)}, \qquad \tilde{\gamma}_j(z) - \gamma_j(z) = \mathscr{O}(|z|^{q-j}), \quad j = 0 \ldots k-1.$$

Then,

$$\begin{aligned}\tilde{\gamma}_k(z) &= z^{-1}\Big(\sum_{j=0}^{k-1} \frac{\tilde{P}_j(z)}{(k-j)\,z^{j+1}Q(z)} - 1\Big) = \sum_{j=0}^{k-1} \frac{\tilde{P}_j(z)}{(k-j)\,z^{j+2}\,Q(z)} - \frac{z^k Q(z)}{z^{k+1}Q(z)} \\ &= \sum_{j=0}^{k-1} \frac{z^{k-j-1}\frac{\tilde{P}_j(z)}{k-j} - z^k Q(z)}{z^{k+1}Q(z)} =: \frac{\tilde{P}_k(z)}{z^{k+1}\,Q(z)}\,,\end{aligned}$$

and

$$\tilde{\gamma}_k(z) - \gamma_k(z) = z^{-1}\sum_{j=0}^{k-1} \frac{\tilde{\gamma}_j(z) - \gamma_j(z)}{k-j} = \sum_{j=0}^{k-1} \mathscr{O}(|z|^{q-j-1}) = \mathscr{O}(|z|^{q-k}).$$

The $\tilde{\gamma}_k(z)$ are well-defined for $z \to 0$ up to $k = p-1$ provided $q \geq p-1$. □

Corollary 3.1 *Under Assumption 3.1, the $\tilde{\gamma}_k(z)$, $k = 0 \ldots p-1$, are of the form*

$$\tilde{\gamma}_k(z) = \frac{P_k(z)}{Q(z)}, \quad k = 0 \ldots p-1, \tag{3.7}$$

with certain polynomials $P_k(z)$, and $Q(z)$ from (3.1).

Proof The assertion follows from Lemma 3.1, observing that (3.5),(3.6) imply

$$\tilde{P}_k(z) = z^{k+1}Q(z)\gamma_k(z) + \mathscr{O}(|z|^p) \quad \text{for} \;\; z \to 0, \quad k = 0 \ldots p-1.$$

Thus, the $\tilde{P}_k(z)$ have at least a $(k+1)$-fold zero at $z = 0$, and representation (3.7) is valid with the well-defined polynomials $P_k(z) = z^{-k-1}\tilde{P}_k(z)$. □

With (3.7), the scheme (3.2) can also be written in the form

$$Q(Z)\,\tilde{u}_{n+1} = P(Z)\,\tilde{u}_n + h\sum_{k=0}^{p-1} P_k(Z)(\nabla^k \tilde{G}_n)_n. \tag{3.8}$$

The coefficients of $Q(z), P(z)$ and the $P_k(z)$ can easily be precomputed on the basis of recursion (3.4), in contrast to the transcendental functions $\gamma_k(z)$ in the exponential version, for which a more careful implementation for $z \to 0$ is required.

Our convergence analysis in Sect. 4 will rely on the close relationship with exponential Adams methods, making use of appropriate estimates for the difference

$$\delta(Z) = R(Z) - \mathrm{e}^Z, \tag{3.9}$$

and related operators.

3.3 Adams-Padé methods

If $R(z) = \frac{P(z)}{Q(z)}$ is chosen as an A-acceptable[2] Padé approximation to e^z of appropriate order, we call the scheme defined by (3.2) an Adams-Padé method. It is well-known that the Padé(μ,ν) approximation $R(z) = R_{\mu,\nu}(z)$ to e^z is A-acceptable iff $\nu - 2 \leq \mu \leq \nu$, see [7, Theorem 4.12]. In this case, for A satisfying Assumption 1.1 (a), $Q(Z)$ is invertible, $\|Q^{-1}(Z)\|$ is uniformly bounded, and [3]

$$\|R(Z)\| \leq 1 \tag{3.10}$$

for all $h > 0$. In particular, we will consider the L-stable subdiagonal case in more detail, i.e., $R(z) = R_{\mu,\nu}(z)$ with $(\mu,\nu) = (p-2,p-1)$ or $(p-1,p)$. In this cases Assumption 3.1 is satisfied, with classical order $q = 2p-3$ or $q = 2p-1$, respectively.

3.4 Relationship with prior work

In [14] it is demonstrated that the class of methods defined in Sect. 3.1 is equivalent to the class suggested in [20], and it is closely related to similar approaches, see [2, 13, 17, 19]. In most of these papers, variable step size is admitted. In our context, the basic construction is of course the same for variable h, but a representation similar to (3.3),(3.4) will become formally more involved.

A further look at [2, 13, 17, 20, 19] shows that no convergence theory for stiff problems is provided in these papers. Moreover, it has been shown in [14] that some of these versions, while consistent of order p in the classical sense, show a significant order reduction in the stiff case.

The advantage of our point of view is that, at least for constant h, the coefficients of the method are defined by a simple, explicit recursion mimicing the analogous recursion for the exponential integrator. This close relationship with exponential methods enables us to prove a convergence result for Adams-Padé methods in Sect. 4. In particular, this can be seen as a stiff convergence theory for a subclass of the methods proposed in [20].

Example 3.1 (see [20]): Choose $p = 3$, with

$$R(z) = R_{1,2}(z) = \frac{P(z)}{Q(z)} = \frac{1 + \frac{1}{3}z}{1 - \frac{2}{3}z + \frac{1}{6}z^2},$$

the subdiagonal Padé (1,2) approximation to e^z. In this case, the $P_k(z)$ from (3.7) evaluate to

$$P_0(z) = 1 - \tfrac{1}{6}z, \quad P_1(z) = \tfrac{1}{2} - \tfrac{1}{6}z, \quad P_2(z) = \tfrac{5}{12} - \tfrac{1}{6}z.$$

Reformulating the scheme as in [20] (in terms of pointwise evaluations of G_n instead of backward differences) it is easy to see that we exactly obtain the same scheme as in the example from [20, Sect. 5]. In the terminology of [20], this corresponds to the preferred choice $\varepsilon_j(z) \equiv 0$. Also for general p, this choice precisely reproduces our method, see [14].

2 A-acceptable means $|R(z)| \leq 1$ for all $\operatorname{Re} z \leq 0$.

3 This follows from [7, Corollary 11.4].

4 Convergence of Adams-Padé methods

In Sect. 4.1 and 4.2 we prove auxiliary results which will be used in the convergence proof in Sect. 4.3.

4.1 Reformulation of the schemes in terms of derivatives of the nonlinear part

Consider the recursions (2.1),(3.2) for the exponential and rational integrators. We are assuming that Assumption 3.1 hold, such that the rational integrator is well-defined. The multistep parts in the schemes involve sums of the form

$$\sum_{k=0}^{p-1} \gamma_k(Z)(\nabla^k G_n)_n, \qquad \sum_{k=0}^{p-1} \tilde{\gamma}_k(Z)(\nabla^k \tilde{G}_n)_n, \tag{4.1}$$

where the $G_n(t)$ and $\tilde{G}_n(t)$ are polynomials of degree $\leq p-1$. For the convergence analysis of the rational integrator, it turns out to be convenient to express this in terms of derivatives of $\tilde{G}_n$ rather in than backward differences. Such a reformulation is derived in the sequel.

Let us first consider a sum of the first type in (4.1). Let $f(t)$ be any polynomial of degree $\leq p-1$, satisfying $\nabla^k f \equiv 0$ for $k \geq p$. Thus,[4]

$$\sum_{k=0}^{p-1} \gamma_k(Z)\nabla^k f = \sum_{k\geq 0} \gamma_k(Z)\nabla^k f = \Gamma(\nabla;Z)f,$$

with $\Gamma(\cdot\,;z)$ from (2.3). To derive an alternative representation for $\Gamma(\nabla;Z)f$, we use the explicit form of $\Gamma(\cdot\,;z)$ from (2.3) and use operational calculus[5] to evaluate $\Gamma(\nabla;Z)$. First we consider $\Gamma(\nabla;z)$ for $\nabla\colon f \to \nabla f$ and the multiplication operator $f \to zf$ applied to scalar analytic functions f.

In the following, D denotes the operator representing the first derivative, multiplied by the step size h,[6]

$$Df(t) = hf'(t). \tag{4.2}$$

Note that $\nabla = I - \mathrm{e}^{-D}$. Furthermore, $\Delta = \mathrm{e}^{D} - I$ denotes the forward difference operator.

Let

$$\Gamma_*(\zeta;z) = \frac{\mathrm{e}^z - \mathrm{e}^\zeta}{z-\zeta}\,. \tag{4.3}$$

[4] For notational simplicity, we suppress the grid index n in this section.

[5] Cf., e.g., [5]. Representation (4.4) below may be considered as an abstract version of the variation-of-constants formula. A direct, elementary verification of (4.5) would be rather cumbersome. We also note that a similar relation appears in [15, Lemma 1.1.1].

[6] This denotation is consistent with the notation Z,∇,Δ for the other h-dependent operators involved, avoiding abundance of indices.

Lemma 4.1 *$\Gamma(\nabla;z)$ satisfies*

$$\Gamma(\nabla;z) = \sum_{k\geq 0} \gamma_k(z)\nabla^k = \Gamma_*(D;z), \quad \textit{with} \quad \Gamma_*(\,\cdot\,;z) \ \textit{from (4.3)}. \tag{4.4}$$

If $f(t)$ is a polynomial of degree $\leq p-1$, then

$$\sum_{k=0}^{p-1} \gamma_k(Z)\nabla^k f = \Gamma_*(D;z)f = \gamma_0(z)\sum_{j=0}^{p-1} z^{-j}D^j f - \sum_{j=1}^{p-1} z^{-j}(\Delta D^{j-1})f, \tag{4.5}$$

with $\gamma_0(z) = z^{-1}(\mathrm{e}^z - 1)$.

Proof From (2.3) and with $\log(I-\nabla) = -D$ we have

$$\Gamma(\nabla;z) = \frac{\mathrm{e}^z\,(I-\nabla-\mathrm{e}^{-z})}{(I-\nabla)(z+\log(I-\nabla))} = \frac{\mathrm{e}^z\,(\mathrm{e}^{-D}-\mathrm{e}^{-z})}{\mathrm{e}^{-D}(z-D)} = \frac{\mathrm{e}^z-\mathrm{e}^D}{z-D}\,,$$

which gives (4.4). This expands into

$$\frac{\mathrm{e}^z-\mathrm{e}^D}{z-D} = \Big(\frac{\mathrm{e}^z-I}{z} - \frac{\mathrm{e}^D-I}{z}\Big)\frac{I}{I-z^{-1}D} = (\gamma_0(z) - z^{-1}\Delta)\sum_{j\geq 0} z^{-j}D^j.$$

For $f(t) =$ polynomial of degree $\leq p-1$ we obtain

$$\Gamma(\nabla;z)f = (\gamma_0(z) - z^{-1}\Delta)\sum_{j=0}^{p-1} z^{-j}D^j f = \gamma_0(z)\sum_{j=0}^{p-1} z^{-j}D^j f \,-\, \sum_{j=1}^{p} z^{-j}(\Delta D^{j-1})f.$$

With $(\Delta D^{j-1})f = 0$ for $j = p$, this gives (4.5). □

Actually, we are interested in an analogous relation for the second, 'rational' sum in (4.1). To this end, let $\tilde\Gamma(\zeta;z)$ and $\tilde\Gamma_*(\zeta;z)$ be defined analogously to (2.3) and (4.3),

$$\tilde\Gamma(\zeta;z) = \frac{(1-\zeta)R(z)-1}{(1-\zeta)(z+\log(1-\zeta))}\,, \qquad \tilde\Gamma_*(\zeta;z) = \frac{R(z)-\mathrm{e}^\zeta}{z-\zeta}\,. \tag{4.6}$$

With these definitions, the analog of Lemma 4.1 holds true:

Lemma 4.2 *$\tilde\Gamma(\nabla;z)$ satisfies*

$$\tilde\Gamma(\nabla;z) = \sum_{k\geq 0} \tilde\gamma_k(z)\nabla^k = \tilde\Gamma_*(D;z), \quad \textit{with} \quad \tilde\Gamma_*(\,\cdot\,;z) \ \textit{from (4.6)}. \tag{4.7}$$

If $f(t)$ is a polynomial of degree $\leq p-1$, then

$$\sum_{k=0}^{p-1} \tilde\gamma_k(Z)\nabla^k f = \tilde\Gamma_*(D;z)f = \tilde\gamma_0(z)\sum_{j=0}^{p-1} z^{-j}D^j f - \sum_{j=1}^{p-1} z^{-j}(\Delta D^{j-1})f, \tag{4.8}$$

with $\tilde\gamma_0(z) = z^{-1}(R(z) - 1)$.

Proof $\tilde{\Gamma}(\zeta;z)$ is of the same form as $\Gamma(\zeta;z)$, with coefficient $R(z)$ instead of e^z, and the same assertion is true for the derivatives of these functions w.r.t. ζ, and for their series expansions about $\zeta = 0$. Therefore, comparing the definition of the $\gamma_k(z)$ (cf. (2.4),(2.5)) and of $\tilde{\gamma}(z)$ (cf. (3.3),(3.4)) we see that, analogously to (2.3), $\tilde{\Gamma}(z)$ expands into

$$\tilde{\Gamma}(\zeta;z) = \sum_{k\geq 0} \tilde{\gamma}_k(z)\zeta^k,$$

i.e., $\tilde{\Gamma}(\zeta;z)$ is the generating function for the $\tilde{\gamma}(z)$. Consequently, *mutatis mutandis*, all conclusions from the proof of Lemma 4.1 hold true. □

Corollary 4.1 *For $Z \in \mathbb{C}^{d\times d}$ instead of $z \in \mathbb{C}$, the conclusions of Lemmas 4.1 and 4.2 remain valid.*

Proof The operational calculus used in the proof of Lemmas 4.1 and 4.2 remains valid for the higher-dimensional case, because all appearing operators D, ∇, Δ commute with evaluation of the constant matrix Z. □

These results show that (2.1) and (3.2) can be written in the form

$$u_{n+1} = \mathrm{e}^Z u_n + h\,\gamma_0(Z)G_n + h\sum_{j=1}^{p-1} Z^{-j}\big[\gamma_0(Z)(D^j G_n)_n - (\Delta D^{j-1}G_n)_n\big], \tag{4.9}$$

$$\tilde{u}_{n+1} = R(Z)\tilde{u}_n + h\,\tilde{\gamma}_0(Z)\tilde{G}_n + h\sum_{j=1}^{p-1} Z^{-j}\big[\tilde{\gamma}_0(Z)(D^j \tilde{G}_n)_n - (\Delta D^{j-1}\tilde{G}_n)_n\big]. \tag{4.10}$$

4.2 The error of Padé approximations to the matrix exponential

For the error of Padé approximations to e^z, the following error estimate dates back to [18] (see also [9, p. 241], [16]):

Lemma 4.3 *Let $R(z) = R_{\mu,\nu}(z) = \frac{P(z)}{Q(z)}$ be the Padé(μ,ν) - approximation to e^z, with $P(0) = Q(0) = 1$. Then,*

$$P(z) - \mathrm{e}^z Q(z) = \frac{(-1)^{\nu+1}}{(\mu+\nu)!} z^{\mu+\nu+1}\int_0^1 K_0(\theta)\,\mathrm{e}^{\theta z}\,\mathrm{d}\theta, \quad K_0(\theta) = (1-\theta)^\mu \theta^\nu. \tag{4.11}$$

This extends to a 'lower order Perron representation', and it is also valid for the matrix case:

Corollary 4.2 *For $Z \in \mathbb{C}^{d\times d}$, the Padé$(\mu,\nu)$ - approximation $R(Z) = R_{\mu,\nu}(Z) = \frac{P(Z)}{Q(Z)}$ to e^Z, with $P(0) = Q(0) = I$, satisfies*

$$P(Z) - \mathrm{e}^Z Q(Z) = \frac{(-1)^{\nu+1-\ell}}{(\mu+\nu)!} Z^{\mu+\nu+1-\ell}\int_0^1 K_\ell(\theta)\,\mathrm{e}^{\theta Z}\,\mathrm{d}\theta \tag{4.12}$$

for $0 \leq \ell \leq \min\{\mu,\nu\}$, with kernel polynomials $K_\ell(\theta) = \frac{\mathrm{d}^\ell}{\mathrm{d}\theta^\ell}\big((1-\theta)^\mu\theta^\nu\big)$.

Proof First we consider the scalar case $Z = z \in \mathbb{C}$. The kernel $K_0(\theta)$ in (4.11) has a ν-fold zero at $\theta = 0$ and a μ-fold zero at $\theta = 1$. Performing $\ell \leq \min\{\mu, \nu\}$ steps of partial integration, where the kernel polynomial is successively differentiated and the exponential term is integrated, shows (4.12) because, due to

$$\frac{\mathrm{d}^j}{\mathrm{d}\theta^j}\big((1-\theta)^\mu\,\theta^\nu\big) = 0 \quad \text{at } \theta = 0,\ \theta = 1, \quad \text{for } 0 \leq j < \ell,$$

all occurring boundary terms vanish.

For $Z = z \in \mathbb{C}$, the left as well as the right-hand side of (4.12) are entire functions in z and they are identical. Thus, the validity of (4.12) for $Z \in \mathbb{C}^{d\times d}$ immediately follows from the theory of matrix functions, see, e.g., [9, Theorem 1.14]. □

Corollary 4.3 *Let $R(z) = R_{\mu,\nu}(z)$, $\nu - 2 \leq \mu \leq \nu$, be an A-acceptable Padé approximation to e^z (see Sect. 3.3). Then, for $Z = hA$ satisfying Assumption 1.1 (a), $\delta(Z)Z^{-m} = (R(Z) - \mathrm{e}^Z)Z^{-m}$ is well-defined and uniformly bounded,*

$$\|\delta(Z)Z^{-m}\| \leq C \quad \textit{for } m = 0\ldots\mu+\nu+1, \tag{4.13}$$

with certain constants C independent on Z.

Proof First we consider $Z = z \in \mathbb{C}$ with $\operatorname{Re} z \leq 0$. $Q(z)$ has degree ν and its inverse is uniformly bounded.

- For $m = 0$, the uniform estimate $\|\delta(z)\| \leq C_0 = 2$ is obvious.
- For $1 \leq m \leq \mu$ we use (4.12) to write $\delta(z)$ in the form

  $$\delta(z) = Q^{-1}(z)z^{\mu+\nu+1-\ell}E_\ell(z), \quad 0 \leq \ell \leq \mu,$$

  with a function $E_\ell(z)$ satisfying $\|E_\ell(z)\| \leq C$. Choosing ℓ according to $0 < \ell = \mu + 1 - m \leq \mu$ we obtain

  $$\delta(z)z^{-m} = Q^{-1}(z)z^\nu z^{\mu+1-\ell-m}E_\ell(z) = Q^{-1}(z)z^\nu E_\ell(z),$$

  where $Q^{-1}(z)z^\nu$ is uniformly bounded for $\operatorname{Re} z \leq 0$ (use maximum principle).
- For $\mu + 1 \leq m \leq \mu+\nu+1$ we use (4.12) with $\ell = 0$,

  $$\delta(z)z^{-m} = Q^{-1}(z)z^{\mu+\nu+1-m}E_\ell(z),$$

  where $0 \leq \mu+\nu+1-m \leq \nu$, which is also be seen to be bounded for $\operatorname{Re} z \leq 0$ via the maximum principle.

This shows (4.13) for the scalar case. The analogous assertion for $Z \in \mathbb{C}^{d\times d}$ follows by from [7, Corollary 11.4] and observing that the $\|E_\ell(Z)\|$ are also uniformly bounded. □

4.3 Convergence for semilinear problems

In the convergence theorem we assume that $R(z)$ is a subdiagonal Padé approximation. Two versions are considered.[7]

Theorem 4.1 *Let the initial value problem (1.2) satisfy Assumption 1.1, and consider for its numerical solution the p-step Adams-Padé method (3.2) with step size h satisfying* $0 < h < H$ *with H sufficiently small. In particular, let*

$$\text{(i)}\;\; R(z) = \textit{Padé}\,(p-2, p-1), \;\; p \geq 3, \quad \textit{or}$$
$$\text{(ii)}\;\; R(z) = \textit{Padé}\,(p-1, p), \;\; p \geq 2.$$

Let $f(t) = g(t, u(t))$ *and assume that* $f \in C^p([0,T], \mathbb{C}^d)$. *Then, for*

$$\|\tilde{u}_n - u(t_n)\| \leq \tilde{c}_0\, h^p, \quad n = 0 \ldots p-1, \tag{4.14}$$

the error bound

$$\|\tilde{u}_n - u(t_n)\| \leq C\, \tilde{c}_0\, h^p + \tilde{C}\, h^p \sup_{0 \leq t \leq t_n} \big(\, \|u^{(p+1)}(t)\| + \|f^{(p)}(t)\|\,\big) \tag{4.15}$$

holds uniformly for $0 \leq nh \leq T$. *The constant* $\tilde{C}$ *depends on T, but is independent of n and h.*

Proof

- *Preparation.* First we note that the uniform estimates
$$\|\delta(Z) Z^{-(j+1)}\| \leq C, \quad j = 0 \ldots p, \tag{4.16}$$
follow from Corollary 4.3 in both cases considered, because $p+1 \leq \mu + \nu + 1 = 2p-2$ for $p \geq 3$ (case (i)), and $p+1 \leq \mu + \nu + 1 = 2p$ for $p \geq 2$ (case (ii)).
- *Induction for global error.* With the notation introduced in Sections 3 and the present section, we consider the recursion for the $\tilde{u}_n$ in the form (4.10),
$$\tilde{u}_{n+1} = R(Z)\tilde{u}_n + h \sum_{j=0}^{p-1} Z^{-j} \tilde{\gamma}_0(Z) (D^j\, \tilde{G}_n)_n - h \sum_{j=1}^{p-1} Z^{-j} (\Delta D^{j-1} \tilde{G}_n)_n.$$
With $f_n = f(t_n) = g(t_n, u(t_n))$, and
$$F_n(t) = \text{Lagrange interpolant of degree } p-1 \text{ at } \; (t_{n-k}, f_{n-k}), \; k = 0 \ldots p-1,$$
the local truncation error of $u(t)$ w.r.t. the rational Adams scheme is given by
$$\tilde{\tau}_{n+1} = u(t_{n+1}) - R(Z) u(t_n) - h \sum_{j=0}^{p-1} \tilde{\gamma}_0(Z) Z^{-j} (D^j F_n)_n + h \sum_{j=1}^{p-1} Z^{-j} (\Delta D^{j-1} F_n)_n,$$
and the global error $\tilde{e}_n = \tilde{u}_n - u(t_n)$ satisfies the recursion
$$\tilde{e}_{n+1} = R(Z)\tilde{e}_n + h \sum_{j=0}^{p-1} \delta(Z) Z^{-(j+1)} [(D^j\, \tilde{G}_n)_n - (D^j F_n)_n] - \tilde{\tau}_{n+1}. \tag{4.17}$$

[7] $p = 2$ with $R(z) = \text{Padé}\,(0,1)$ is a special case, with a reduced convergence order $p-1 = 1$. An analogous convergence result can be derived for the diagonal Padé case.

– *Estimation of nonlinear terms.* With (4.2) we have

$$(D^j\,\tilde G_n)_n-(D^jF_n)_n=h^j\,(\tilde G^{(j)}(t_n)-F_n^{(j)}(t_n))=h^j\,\psi_n^{(j)}(t_n),\qquad(4.18)$$

where $\psi_n(t)$ denotes the Lagrange interpolant of degree $p-1$ at

$$\big(t_{n-k},g(t_{n-k},\tilde u_{n-k})-g(t_{n-k},u(t_{n-k}))\big),\;\; k=0\ldots p-1.$$

The j-th derivative of the polynomial $\psi_n(t)$ at $t=t_n$ can be written as a weighted sum of the form

$$\psi_n^{(j)}(t_n)=h^{-j}\sum_{m=j}^{p-1}C_{j,m}\,h^m(\nabla^m\Psi_n)_n,$$

with certain fixed weights $C_{j,m}$ (cf., e.g., [12]). Using the Lipschitz continuity of g (Assumption 1.1 (b)),(4.18) can thus be estimated by

$$\|(D^j\,\tilde G_n)_n-(D^jF_n)_n\|\le C\sum_{j=1}^{p}\|\tilde u_{n-p+j}-u(t_{n-p+j})\|=C\sum_{j=1}^{p}\|\tilde e_{n-p+j}\|.\quad(4.19)$$

– *Representation and estimation of local truncation error.* In order to estimate $\tilde\tau_{n+1}$, we first consider the truncation error τ_{n+1} with respect to the exponential scheme (4.9) which has a form analogous to $\tilde\tau_{n+1}$. With $\delta(Z)=R(Z)-\mathrm{e}^Z$ and $\tilde\gamma_0(Z)-\gamma_0(Z)=Z^{-1}\delta(Z)$, this gives

$$\tilde\tau_{n+1}=\tau_{n+1}-\delta(Z)u(t_n)-h\sum_{j=0}^{p-1}\delta(Z)Z^{-(j+1)}(D^jF_n)_n.$$

For τ_{n+1} it is easy to show that

$$\|\tau_{n+1}\|\le C\,h^{p+1}\sup_{0\le t\le t_{n+1}}\|f^{(p)}(t)\|,\qquad(4.20)$$

see [10, Theorem 4.2]. Furthermore, with (4.2) we have

$$(D^jF_n)_n=h^j\,F_n^{(j)}(t_n)=h^j\,f^{(j)}(t_n)+h^j\,\rho_n^{(j)},$$

with

$$\|\rho_n^{(j)}\|=\|(F_n^{(j)}-f^{(j)})(t_n)\|\le C\,h^{p-j}\sup_{0\le t\le t_n}\|f^{(p)}(t)\|,\qquad(4.21)$$

for $j=0\ldots p-1$. Denoting

$$\sigma_{n+1}=\sum_{j=0}^{p-1}\delta(Z)Z^{-(j+1)}h^{j+1}\rho_n^{(j)},$$

and making use of (1.2) we can now write $\tilde{\tau}_{n+1}$ in the form

$$\begin{aligned}\tilde{\tau}_{n+1} &= -\delta(Z)\Big[u(t_n) + \sum_{j=0}^{p-1} Z^{-(j+1)} h^{j+1} f^{(j)}(t_n)\Big] + \tau_{n+1} - \sigma_{n+1} \\ &= -\delta(Z) Z^{-(p+1)}\, h^{p+1} \underbrace{\Big[A^{p+1}\, u(t_n) + \sum_{j=0}^{p-1} A^{p-j} f^{(j)}(t_n)\Big]}_{=\, A\, u^{(p)}(t_n)} + \tau_{n+1} - \sigma_{n+1} \\ &= -\delta(Z) Z^{-(p+1)}\, h^{p+1}\big[u^{(p+1)}(t_n) - f^{(p)}(t_n)\big] + \tau_{n+1} - \sigma_{n+1}, \qquad (4.22)\end{aligned}$$

Here, $\tau_{n+1} = \mathscr{O}(h^{p-j})$ is bounded according to (4.20), and σ_{n+1} satisfies

$$\|\sigma_{m+1}\| \leq \sum_{j=0}^{p-1} \|\delta(Z) Z^{-(j+1)}\|\, h^{j+1}\, \|\rho_n^{(j)}\|, \qquad (4.23)$$

with $\rho_n^{(j)} = \mathscr{O}(h^{p-j})$ bounded according to (4.21).

- *Estimation of global error.* Eventually, from (4.20)–(4.23) together with (4.16),(4.17) and (4.19) we conclude that for $n \geq p$ the global error $\tilde{e}_n$ satisfies

$$\begin{aligned}\|\tilde{e}_{n+1}\| &\leq \|R(Z)\|\, \|\tilde{e}_n\| + \\ &+ Ch \sum_{j=1}^{p} \|\tilde{e}_{n-p+j}\| + C h^{p+1} \sup_{0 \leq t \leq t_n} \big(\, \|u^{(p+1)}(t)\| + \|f^{(p)}(t)\|\,\big).\end{aligned}$$

With starting values according to (4.14) and due to (3.10), the result (4.15) now follows in a standard way by application of the discrete Gronwall Lemma. □

5 Numerical example; discussion

For illustration of our results we consider the same test problem as in [11, Sect. 4],

$$U_t(x,t) = U_{xx}(x,t) + \frac{1}{1 + U(x,t)^2} + \Phi(x,t), \qquad (5.1)$$

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 (5.1) in space by standard finite differences using an equidistant mesh Δ_x with 200 inner mesh points x_i. This yields a stiff initial value problem of the form (1.2) with exact semi-discrete solution $U_\Delta(x_i,t) \equiv U(x_i,t)$.

We integrate the system in time with the p-step Adams-Padé methods for $p = 2 \ldots 6$, with $R(z) = \text{Padé}\,(p-2, p-1)$, except $p = 2$ where we have used Padé $(1,1)$. We compute the errors in a discrete L^2 norm. The results which are displayed in Fig. 5.1 in a double-logarithmic diagram. They are in perfect agreement with Theorem 4.1 and should be compared with the results from [11], which are very similar.

These numerical results have been obtained by implementing (3.2) using straightforward diagonalization of the finite-difference matrix A, evaluating the orthogonal

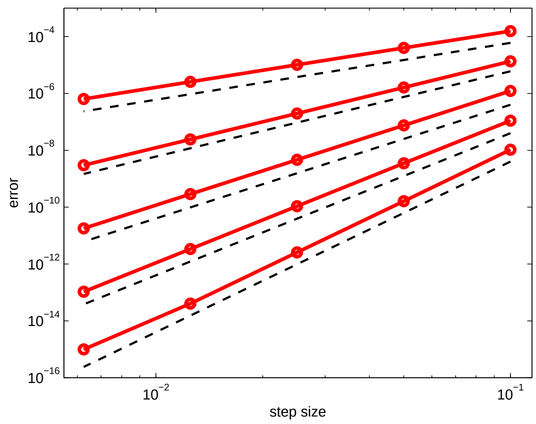

Fig. 5.1 Order plots for the p-step Adams-Padé methods ($p = 2 \ldots 6$) applied to example (5.1). The problem is discretized in space with 200 mesh points and integrated in time with constant step sizes. The dashed lines are straight lines of slope p.

transformations involved via discrete sine transforms. For more challenging problems or when using a linearized version (1.4), ways for efficient implementation have to be considered. Basically, the techniques as described in [11, Sect. 5] apply also in the present context, e.g. how to compute accurate starting values.

Remark 5.1 In contrast to exponential schemes, each step of the rational version is equivalent to the solution a linear system with coefficient matrix $Q(Z)$, see (3.8), which appears to be advantageous. However, in typical applications, these linear systems tend to be very ill-conditioned for fine spatial meshes and higher order p. In the above example, for instance, Cholesky elimination fails to produce double precision accuracy for $p \geq 4$.

However, the fact that linear systems are involved should not be underestimated, because many solution techniques can potentially be applied, e.g. of multilevel type. A topic worth considering will be the use of Krylov subspace methods. These are well-established techniques for the approximation of the matrix exponential and the φ_j- or γ_k-functions, see [9, 10] and references therein. Using Padé approximations for computing the matrix exponential in the reduced subspace is a common technique, see [9]. On the other hand, aiming to approximate a given $R(Z)$ directly, instead of e^Z, we remain in a completely linear setting. Solution of the reduced problem and, in particular, evaluation or estimation of the subsequent, appropriately scaled residual may well benefit from the linear structure. These questions, and other topics as for instance variable step size versions and further pros/cons in relation to exponential schemes are subject to further, more implementation-oriented studies.

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