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Exponential fitted Runge–Kutta methods of collocation type: fixed or variable knot points?

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Abstract

Two different classes of exponential fitted Runge–Kutta collocation methods are considered: methods with fixed points and methods with frequency-dependent points. For both cases we have obtained extensions of the classical two-stage Gauss, RadauIIA and LobattoIIIA methods. Numerical examples reveal important differences between both approaches.

MSC: 65L05

Keywords: Runge–Kutta methods; Exponential fitting; Oscillating differential equations

1. Introduction

Many phenomena exhibit a pronounced oscillatory or exponential character. The theoretical investigation of such phenomena necessarily implies operations on oscillatory or exponential functions, for instance differentiation, quadrature, solving differential equations, etc. In a previous paper [8] Ixaru had focussed on the numerical formulae associated with these operations. He showed that a unifying treatment for deriving formulae for differentiation, quadrature and ODEs is available in the form of exponential fitting. In the context of ODEs he only introduced the method for the determination of multistep-like formulae. In this paper, we extend the technique to Runge–Kutta (RK) methods.

Quite some exponential fitted RK (EFRK) methods have been constructed so far. In the mid-eighties van der Houwen et al. constructed RK (–Nyström) methods with a reduced or null phase error [19–21]. Recently several authors [5,11–13] have constructed RK (–Nyström) methods for which they claim that trigonometric functions with known periodicity are integrated exactly. Paternoster

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[12] used the linear stage representation of an RK method given in Albrecht's approach and derived some examples of implicit RK (–Nyström) methods of low algebraic order (for the definition of this property see [12]). On the other hand, Simos [13] constructed an explicit RK method of algebraic order 4, which exactly integrates certain first-order initial value problems with periodic or exponential solutions. Simos [3,14,15] applied some modified RK methods to solve Schrödinger equations. In [16] a more general explicit RK method of algebraic order 4, which integrates exactly first-order systems with solutions which can be expressed as linear combinations of $\exp(\omega x)$ and $\exp(-\omega x)$ (ω may be either real or purely imaginary), is constructed and applied on several test systems. The present authors studied some specific EFRK methods [17,18].

The procedures used in all these papers for deriving EFRK methods look very much distinct. As already mentioned, here we shall show how the derivation of such formulae can be covered by the techniques, analogous to the one introduced by Ixaru [8].

The paper is organized as follows. In Section 2, we establish the main elements of the approach. This is further applied for deriving specific two stage EFRK schemes in Section 3. In particular, we construct several exponential fitted versions of well-known classical collocation methods. These methods can be divided into two categories: methods with fixed knot points and methods with variable knot points. From a theoretical point of view, the construction of both classes is quite similar; however, the numerical examples in Section 4 reveal important differences. In Section 5, an analysis of this different behaviour is made. Finally, in Section 6 some conclusions are drawn.

2. Basic elements of the approach

For the description of EFRK methods we use the classical Butcher notation [4,10]

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \tag{2.1}$$

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) \tag{2.2}$$

with $i = 1, \ldots, s$, or in tableau form

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \ldots & a_{1s} \\ c_2 & a_{21} & a_{22} & \ldots & a_{2s} \\ & & \ldots & & \\ c_s & a_{s1} & a_{s2} & \ldots & a_{ss} \\ \hline & b_1 & b_2 & \ldots & b_s \end{array} \tag{2.3}$$

Following Albrecht's approach [1,2,10] we observe that each of the s internal stages (2.2) and the final stage (2.1) of an RK-method are linear, in the sense that a linear multistep method is linear. Nonlinearity only arises when one substitutes from one stage into another. We can regard each of the s stages and the final stage as being a generalized linear multistep method on a nonequidistant grid and associate with it a linear functional in exactly the same way as has been done by Ixaru [8] for multistep methods, i.e.,

$$\mathscr{L}_i[y(x);h;\mathbf{a}] = y(x+c_ih) - y(x) - h\sum_{j=1}^{s} a_{ij}y'(x+c_jh) \quad i=1,2,\ldots,s \tag{2.4}$$

and

$$\mathscr{L}[y(x);h;\mathbf{b}] = y(x+h) - y(x) - h\sum_{i=1}^{s} b_iy'(x+c_ih). \tag{2.5}$$

If one considers for y a set of power functions, i.e.,

$$1, x, x^2, x^3, \ldots,$$

all functionals in this paper can be rewritten as [8]

$$\mathscr{L}_i[y(x);h;\mathbf{a}] = L_{i0}(h,\mathbf{a})y + \frac{1}{1!}L_{i1}(h,\mathbf{a})y' + \cdots + \frac{1}{m!}L_{im}(h,\mathbf{a})y^{(m)} + \cdots \tag{2.6}$$

$$\mathscr{L}[y(x);h;\mathbf{b}] = L_0(h,\mathbf{b})y + \frac{1}{1!}L_1(h,\mathbf{b})y' + \cdots + \frac{1}{m!}L_m(h,\mathbf{b})y^{(m)} + \cdots \tag{2.7}$$

where the symbols $L_{ij}(h,\mathbf{a})$ and $L_i(h,\mathbf{b})$ are called moments. They are the expressions for $\mathscr{L}_i[x^j;h;\mathbf{a}]$ and $\mathscr{L}[x^i;h,\mathbf{b}]$ at $x=0$, respectively. When for y a so-called exponential fitting set is introduced, i.e., pairs of exponentials of the form

$$\exp(\pm\omega x), x\exp(\pm\omega x), x^2\exp(\pm\omega x), \ldots$$

the functionals appearing in this paper can be transformed with the aid of the following general form:

$$\mathscr{L}_i[\exp(\omega x);h;\mathbf{a}] = w_i(h)\exp(\omega x)g_i(v,\mathbf{a}), \tag{2.8}$$

$$\mathscr{L}[\exp(\omega x);h;\mathbf{b}] = w(h)\exp(\omega x)g(v,\mathbf{b}), \tag{2.9}$$

where $w_i(h)$ and $w(h)$ are functions of h alone and g_i and g are linear combination of the components of the vectors $\mathbf{a}$ and $\mathbf{b}$, respectively, and $v=\omega h$. The procedure to get tuned formulae follows then the same chain of operations as given by [8].

1. Start with the functionals given and evaluate their moments $L_{ij}(h,\mathbf{a})$, $i=1,\ldots,s$, $j=0,1,2,\ldots$ and $L_i(h,\mathbf{b})$, $i=0,1,2,\ldots$.
2. Examine the linear systems

$$L_{ij}(h,\mathbf{a}) = 0, \quad i=1,\ldots,s;\ j=0,1,2,\ldots,M, \tag{2.10}$$

$$L_i(h,\mathbf{b}) = 0, \quad i=0,1,2,\ldots,M' \tag{2.11}$$

to find out the maximal M and M' values for which they are compatible. In what follows it is obvious to choose $M=s$; the RK-methods related to that choice are the so-called collocation methods with stage order s. For this particular choice M' can vary between s and $2s$. In the latter case the Gauss methods are obtained. From the structure itself of relations (2.1)–(2.2) it is clear that for every $i=1,2\dots,s$

$$L_{i0}(h,\mathbf{a})=0 \quad \text{and} \quad L_0(h,\mathbf{b})=0.$$

In other words a constant is always exactly integrated by an RK method. The conditions $L_{ij}(h,\mathbf{a})=0$, $i=1,\dots,M$, give rise to the equations

$$h^j\left(c_i^j - j\sum_{k=1}^{s} a_{ik}c_k^{j-1}\right)=0, \quad j=1,\dots,s,\ i=1,\dots,M, \tag{2.12}$$

which are the well-known stage-order conditions [4,6,10] or simplifying assumptions denoted as $C(M)$. The $j=1$ case just represents the well-known row-sum condition. The conditions $L_i(h,\mathbf{b})=0$ give rise to the equations

$$h^i\left(1 - i\sum_{j=1}^{s} b_j c_j^{i-1}\right)=0; \quad i=1,\dots,M', \tag{2.13}$$

which represent the order conditions that correspond for each $i\leqslant M'$ to the tree $[\tau^{i-1}]$ in the Butcher theory and are denoted in [6] as $B(M')$. Under the restrictions $M=s$ and $s\leqslant M'<2s$ it is the sufficient condition for the method to have order M'.

3. Construct the formal expressions of

$$G_i^+(Z,\mathbf{a})=\frac{1}{2}[g_i(v,\mathbf{a})+g_i(-v,\mathbf{a})],$$

$$G_i^-(Z,\mathbf{a})=\frac{1}{2v}[g_i(v,\mathbf{a})-g_i(-v,\mathbf{a})], \quad i=1,2,\dots,s$$

$$G^+(Z,\mathbf{b})=\frac{1}{2}\,[g(v,\mathbf{b})+g(-v,\mathbf{b})],$$

$$G^-(Z,\mathbf{b})=\frac{1}{2v}\,[g(v,\mathbf{b})-g(-v,\mathbf{b})] \tag{2.14}$$

with $Z=v^2$ and of their pth-order derivatives with respect to Z denoted $G_i^{\pm(p)}(Z,\mathbf{a})$ and $G^{\pm(p)}(Z,\mathbf{b})$ for $p=1,2,\dots$

4. Choose the reference sets of $M+1$ and $M'+1$ functions which are appropriate for the given form of $y(x)$. This is in general a hybrid set,

$$1,x,x^2,\dots,x^K \text{ or } x^{K'},$$

$$\exp(\pm\omega x), x\exp(\pm\omega x),\dots,x^P\exp(\pm\omega x) \text{ or } x^{P'}\exp(\pm\omega x)$$

with either $K+2P=M-2$ or $K'+2P'=M'-2$. This means that the parameters P or P' and K' or K' can have different values in the internal stages and in the final stage. The two parameters $K(K')$ and $P(P')$ characterize the reference set. The set in which there is no classical component (except for 1) is identified by $K=0$ and $K'=0$ while the set in which there is no exponential fitting component is identified by $P=-1$ and $P'=-1$. The parameters P' and P are called the levels of tuning for the final and internal stages and the best tuned formula will be that which corresponds to the integer values $P=[(M-2)/2]$ for the final stage and $P'=[(M-2)/2]$ for the internal stages. Remark that in contrast to the multistep case [8] the smallest value here attainable for $K(K')$ is 0 and not -1.

5. Solve formally the linear systems

$$L_{ij}(h,\mathbf{a})=0,\;\; G_i^{\pm}(Z,\mathbf{a})=0, \quad G_i^{\pm(p)}(Z,\mathbf{a})=0,\;\; p=1,\dots,P$$

with $i=1,2,\dots,s,\;\; j=1,\dots,K$

$$L_i(h,\mathbf{b})=0,\;\; G^{\pm}(Z,\mathbf{b})=0, \quad G^{\pm(p)}(Z,\mathbf{b})=0,\;\; p=1,\dots,P'$$

with $i=1,2,\dots,K'$,

with Z-dependent coefficients. The numerical values of a_{ij} and b_i are computed either for real ω-values (exponential case) or for pure imaginary ω-values (oscillatory case).

6. Once the Butcher tableau determined, the principal (i.e., leading order) term of the local truncation error (*plte*) can be written down as well as for the pure classical, pure exponential fitted as for the mixed case. Specific examples for the nonautonomous scalar case will be given in Section 3.

3. Two stage collocation methods

In this section, we will discuss the construction of two-stage RK methods and EFRK methods of collocation type, i.e., $M' \geqslant M=s=2$.

3.1. Classical Runge–Kutta methods

We start with $M'=2$. To obtain the classical (i.e., polynomial based) methods, we put $K=K'=2$ and $P=P'=-1$. The solution of the systems $L_{ij}(h,\mathbf{a})=0$ and $L_i(h,\mathbf{b})=0$, $(i=1,2;\;\; j=1,2)$ is then given by

$$a_{11}=\frac{c_1(-c_1+2c_2)}{2(-c_1+c_2)}, \quad a_{12}=-\frac{c_1^2}{2(-c_1+c_2)}, \quad a_{21}=\frac{c_2^2}{2(-c_1+c_2)},$$

$$a_{22}=\frac{c_2(-2c_1+c_2)}{2(-c_1+c_2)}, \quad b_1=\frac{(2c_2-1)}{2(-c_1+c_2)}, \quad b_2=-\frac{(2c_1-1)}{2(-c_1+c_2)}.$$

As well known, a particular choice of c_1 and c_2 determines the order of the method:

- For arbitrary c_i's the order is 2. In particular for $c_1=0$ and $c_2=1$ one obtains the LobattoIIIA method.
- Adding $L_3(h,\mathbf{b})=0$ (this means $M'=3,\;\; K'=3,\;\; P'=-1$) to the equations previously considered we find $c_1=(3c_2-2)/3(2c_2-1)$; the special choice $c_2=1$ (such that $c_1=1/3$) results in the two-stage RadauIIA method.

- Adding $L_3(h,\mathbf{b})=0$ and $L_4(h,\mathbf{b})=0$ (this means $M'=4$, $K'=4$, $P'=-1$) to the equations considered delivers $c_1=(3-\sqrt{3})/6$ and $c_2=(3+\sqrt{3})/6$. Remark that the simplifying assumptions $C(s)$ and the quadrature order conditions $B(2s)$ are fulfilled. Due to the theorem 342A and 342D in [4] one can prove that the so-called $D(s)$ simplifying conditions

$$\sum_{i=1}^{s} b_i c_i^{q-1} a_{ij} = \frac{b_j}{q}(1-c_j^q), \quad j=1,\dots,s;\; q=1,\dots,s$$

are also fulfilled, resulting in the fact that the maximal algebraic order $2s=4$ is obtained. This method is known as the 2-stage Gauss method.

For these classical methods, the plte is well described in [6,10] as

$$\text{plte} = \frac{h^{p+1}}{(p+1)!} \sum_{r(t)=p+1} \alpha(t)[1-\gamma(t)\psi(t)]F(t) \tag{3.1}$$

with p being the order of the method (varying between M and M'); for the explanation of the used symbols we refer to [10].

- In case the order p and the stage order q satisfy $p=M'=s$ and $q=M=s$ it is easy to show that for every occurring t

$$\gamma(t)\psi(t) = \gamma([\tau^{s+1}])\psi([\tau^{s+1}]) \tag{3.2}$$

such that in that case

$$\text{plte} = \frac{h^{s+1}}{(s+1)!}(1-\gamma([\tau^{s+1}])\psi([\tau^{s+1}])) \sum_{r(t)=s+1} \alpha(t)F(t),$$

which simplifies to

$$\text{plte} = \frac{h^{s+1}}{(s+1)!}(1-\gamma([\tau^{s+1}])\psi([\tau^{s+1}]))y^{(s+1)}.$$

For the LobattoIIIA case with $s=2$, this last expression reads

$$\begin{aligned}\text{plte(LobattoIIIA}, s=2) &= \frac{h^3}{3!}\left(1-3\sum_{i=1}^{2} b_i c_i^2\right) y^{(3)} \\ &= -\frac{h^3}{12}\, y^{(3)}. \end{aligned} \tag{3.3}$$

- In the case $p=M'=s+1$ and $q=M=s$ (3.1) does not simplify to a very simple expression, depending only on one total derivative of the solution y. One can use the simplifying assumptions (in fact the moments L_{ij}) to derive the plte expression. For the case $s=2$ one finds

$$\text{plte} = \frac{h^4}{4!}\left[\left(1-4\sum_{i=1}^{2} b_i c_i^3\right) y^{(4)} + \left(4\sum_{i=1}^{2} b_i c_i^3 - 12\sum_{i,j=1}^{2} b_i a_{ij} c_j^2\right) f_y y^{(3)}\right].$$

This expression clearly shows that the methods considered has order 3 and stage order 2. In the case of the RadauIIA method this form reduces to

$$\mathrm{plte}(\mathrm{RadauIIA}, s=2) = -\frac{h^4}{216}(y^{(4)} - 4f_y y^{(3)}). \tag{3.4}$$

- In the same spirit one can construct the plte for a method with $p = M' = s+2$ and $q = M = s$. For $s = 2$ one then has

$$\mathrm{plte} = \frac{h^5}{5!}[A' y^{(5)} + (C' - A') f_y y^{(4)} + [(D' - C') f_y^2 + 4(B' - A')(f_{xy} + f_{yy} f)] y^{(3)}].$$

Herein A', B', C' and D' denote

$$A' = \left(1 - 5\sum b_i c_i^4\right),$$

$$B' = \left(1 - 15\sum b_i c_i a_{ij} c_j^2\right),$$

$$C' = \left(1 - 20\sum b_i a_{ij} c_j^3\right),$$

$$D' = \left(1 - 60\sum b_i a_{ij} a_{jk} c_k^2\right).$$

For the Gauss method with $s = 2$ case this simplifies to

$$\mathrm{plte}(\mathrm{Gauss}, s=2) = \frac{h^5}{4320}(y^{(5)} - 5 f_y y^{(4)} + 10(f_y^2 - (f_{xy} + f_{yy} f)) y^{(3)}). \tag{3.5}$$

3.2. Exponential fitted Runge–Kutta methods

3.2.1. Order 2 methods

In the case of exponential fitting, we put $K = 0 = K'$ and $P = 0 = P'$. This means that no classical component (except for 1) is present in the set of functions that are integrated exactly. We consider the solution $\mathbf{b}$ of the equations $G^{\pm}(Z, \mathbf{b}) = 0$ and the solutions $\mathbf{a}$ of $G_i^{\pm}(Z, \mathbf{a}) = 0$, $i = 1, 2$, i.e.,

$$G^{+}(Z, \mathbf{b}) = \xi(Z) - 1 - Z(b_1 c_1 \eta_0(c_1^2 Z) + b_2 c_2 \eta_0(c_2^2 Z)) = 0, \tag{3.6}$$

$$G^{-}(Z, \mathbf{b}) = \eta_0(Z) - (b_1 \xi(c_1^2 Z) + b_2 \xi(c_2^2 Z)) = 0 \tag{3.7}$$

and

$$G_i^{+}(Z, \mathbf{a}) = \xi(c_i^2 Z) - 1 - Z(a_{i1} c_1 \eta_0(c_1^2 Z) + a_{i2} c_2 \eta_0(c_2^2 Z)) = 0, \tag{3.8}$$

$$G_i^{-}(Z, \mathbf{a}) = c_i \eta_0(c_i^2 Z) - (a_{i1} \xi(c_1^2 Z) + a_{i2} \xi(c_2^2 Z)) = 0 \tag{3.9}$$

for $i = 1, 2$. The functions η_0 and ξ and some of their properties are given in Appendix A. Following results are obtained:

$$D = Z(-\xi(c_1^2 Z) c_2 \eta_0(c_2^2 Z) + c_1 \eta_0(c_1^2 Z) \xi(c_2^2 Z)),$$

$$a_{11} = (\xi(c_1^2 Z)\xi(c_2^2 Z) - \xi(c_2^2 Z) - Z c_1 \eta_0(c_1^2 Z) c_2 \eta_0(c_2^2 Z))/D,$$

$$
\begin{aligned}
a_{12} &= (-\xi(c_1^2 Z)^2 + \xi(c_1^2 Z) + Zc_1^2\eta_0(c_1^2 Z)^2)/D,\\
a_{21} &= (\xi(c_2^2 Z)^2 - \xi(c_2^2 Z) - Zc_2^2\eta_0(c_2^2 Z)^2)/D,\\
a_{22} &= (Zc_1\eta_0(c_1^2 Z)c_2\eta_0(c_2^2 Z) - \xi(c_1^2 Z)\xi(c_2^2 Z) + \xi(c_1^2 Z))/D,\\
b_1 &= (\xi(Z)\xi(c_2^2 Z) - \xi(c_2^2 Z) - \eta_0(Z)Zc_2\eta_0(c_2^2 Z))/D,\\
b_2 &= (\eta_0(Z)Zc_1\eta_0(c_1^2 Z) - \xi(Z)\xi(c_1^2 Z) + \xi(c_1^2 Z))/D. \qquad (3.10)
\end{aligned}
$$

These general expressions reduce to very simple ones for particular values of c_1 and c_2. For example, for the LobattoIIIA knot points $c_1 = 0$ and $c_2 = 1$ following results emerge:

$$a_{11} = 0; \quad a_{12} = 0; \quad a_{21} = a_{22} = b_1 = b_2 = \frac{\xi(Z) - 1}{Z\eta_0(Z)}. \qquad (3.11)$$

As for the error, the differential equation $y^{(3)} - \omega^2 y' = 0$ is the one which has the three functions 1, $\exp(\pm\omega x)$ as its linear independent solutions; therefore the leading term should be of the form

$$\text{plte} = X(-\omega^2 y' + y^{(3)}). \qquad (3.12)$$

The factor X is fixed in terms of (2.7). Indeed the coefficient of y' should be the same in (3.12) and (2.7), i.e.,

$$X = -\frac{1}{\omega^2} L_1(h, \mathbf{b}).$$

For the LobattoIIIA case ($c_1 = 0, c_2 = 1$) this leads to the result:

$$\text{plte}(\text{LobattoIIIA}, s = 2, \exp) = -h^3 \frac{Z\eta_0(Z) + 2 - 2\xi(Z)}{Z^2\eta_0(Z)}(-\omega^2 y' + y^{(3)}). \qquad (3.13)$$

In the limit $\omega \to 0$ (this means implicitly that v or $Z \to 0$) all new formulae tend to the classical formulae. This is not immediately visible from (3.11) and (3.13). However, developing the expressions for the elements of the Butcher array and the plte one obtains

$$b_1 = b_2 = a_{21} = a_{22} = \frac{1}{2} - \frac{1}{24} Z + \frac{1}{240} Z^2 + \mathcal{O}(Z^3)$$

and

$$-\frac{Z\eta_0(Z) + 2 - 2\xi(Z)}{Z^2\eta_0(Z)} = -\frac{1}{12} + \frac{1}{120} Z - \frac{17}{20160} Z^2 + \mathcal{O}(Z^3),$$

such that

$$\text{plte}(\text{LobattoIIIA}, s = 2, \exp) = -\frac{h^3}{12}(-\omega^2 y' + y^{(3)}),$$

which confirms that the method has algebraic order 2.

3.2.2. Order 3 methods

In order to increase the algebraic order two strategies can be followed. One can either introduce into (3.10) the classical constant c_i-values of the corresponding RadauIIA or Gauss methods or one can add one or two additional equations to Eqs. (3.6)–(3.7), by increasing M' up to 3 or 4. In this section, we discuss the case $M' = 3$, in Section 3.2.3 we consider the case $M' = 4$.

Case 1 (*Fixed c-Values*): To obtain methods of algebraic order 3 we introduce $c_1 = \frac{1}{3}$ and $c_2 = 1$ into (3.10). Considering the Taylor expansion with respect to Z one obtains (RadauIIA, case 1):

$$a_{11} = \frac{5}{12} + \frac{25}{1296}Z - \frac{5}{23328}Z^2 + \mathcal{O}(Z^3),$$

$$a_{12} = -\frac{1}{12} + \frac{7}{1296}Z - \frac{31}{116640}Z^2 + \mathcal{O}(Z^3),$$

$$a_{21} = b_1 = \frac{3}{4} + \frac{1}{144}Z + \frac{13}{38880}Z^2 + \mathcal{O}(Z^3),$$

$$a_{22} = b_2 = \frac{1}{4} - \frac{1}{144}Z + \frac{11}{38880}Z^2 + \mathcal{O}(Z^3).$$

To check the algebraic order we consider the classical order conditions (for the case where the row-sum condition is not satisfied) in which we introduce the ω-dependent coefficients; following results are obtained:

$$\sum_i b_i = 1 + \frac{1}{1620}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_i b_i c_i = \frac{1}{2} - \frac{1}{216}Z + \frac{23}{58320}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_{i,j} b_i a_{ij} = \frac{1}{2} + \frac{1}{72}Z + \frac{7}{19440}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_i b_i c_i^2 = \frac{1}{3} - \frac{1}{162}Z + \frac{7}{21870}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_{i,j,k} b_i a_{ij} a_{ik} = \frac{1}{3} + \frac{1}{162}Z + \frac{7}{7290}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_{i,j} b_i a_{ij} c_i = \frac{1}{3} - \frac{1}{2430}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_{i,j,k} b_i a_{ij} a_{jk} = \frac{1}{6} + \frac{11}{648}Z + \frac{13}{58320}Z^2 + \mathcal{O}(Z^3),$$

$$\sum_{i,j} b_i a_{ij} c_j = \frac{1}{6} + \frac{1}{216}Z + \frac{7}{58320}Z^2 + \mathcal{O}(Z^3)$$

confirming the algebraic order 3. For the plte we then find

$$\begin{aligned}&\text{plte(RadauIIA}, s = 2, \text{exp, case 1)}\\ &\quad = -\frac{h^4}{216}(-\omega^2 y^{(2)} + y^{(4)} - 4f_y(-\omega^2 y' + y^{(3)})).\end{aligned} \tag{3.14}$$

Case 2 (ω-*Dependent c-Values*): By considering $M' = 3$, (i.e., $K' = 1,\ P' = 0$) we look for the solution $\mathbf{b}$ of the equations $L_1(h, \mathbf{b}) = 0$, i.e.,

$$L_1(h, \mathbf{b}) = h(b_1 + b_2 - 1) = 0 \tag{3.15}$$

and $G^{\pm}(Z, \mathbf{b}) = 0$, as defined in (3.6), (3.7). Solving this system for b_1 and b_2 we obtain

$$b_1 = \frac{\eta(Z) - \xi(c_2^2 Z)}{\xi(c_1^2 Z) - \xi(c_2^2 Z)}, \quad b_2 = \frac{\xi(c_1^2 Z) - \eta(Z)}{\xi(c_1^2 Z) - \xi(c_2^2 Z)} \tag{3.16}$$

and a transcendental relation in the unknown c's. Defining $d_1 := (c_1 - c_2)/2$ and $d_2 := (c_1 + c_2)/2$ this relation can be written as

$$\eta(d_1^2 Z)(\xi(d_1^2 Z) - (1 - d_2)\eta((1 - d_2)^2 Z) - d_2 \eta(d_2^2 Z)) = 0. \tag{3.17}$$

Guided by the classical RadauIIA case, one can choose either $c_1 = 1/3$ (RadauIIA, case 2a) or $c_2 = 1$ (RaduaIIA, case 2b).

Case 2a ($c_1 = \frac{1}{3}$): Equation (3.17) is now a transcendental equation in c_2. A contourplot as in Fig. 1 (showing where the l.h.s. of (3.17) is equal to zero) reveals that there are several solutions, however, it is the curve passing through $(c_2, Z) = (1, 0)$ which we are interested in. In practice we are interested in that part of the curve for which $|Z|$ is of moderate size (let us say smaller than 5). For such values of Z, one can solve (3.17) explicitly for c_2 to obtain

$$c_2 = \begin{cases} \dfrac{2}{3} + \dfrac{1}{\sqrt{Z}} \log\left(\dfrac{-G_1 + 1 + \sqrt{Z}G_1^{1/3}}{-1 + G_1 - \sqrt{Z}G_1^{2/3}}\right), & Z > 0, \\ 1, & Z = 0, \\ \dfrac{2}{3} - \dfrac{i}{\sqrt{-Z}} \log\left(\dfrac{-G_2 + 1 + i\sqrt{-Z}G_2^{1/3}}{-1 + G_2 - i\sqrt{-Z}G_2^{2/3}}\right), & Z < 0, \end{cases} \tag{3.18}$$

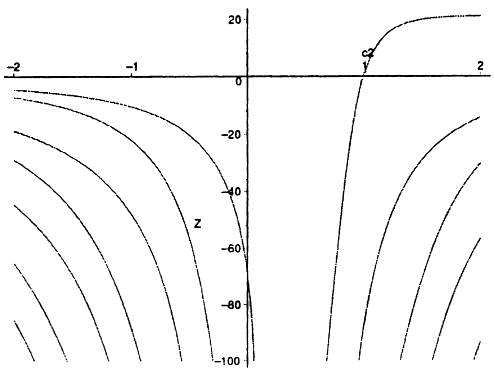

Fig. 1. The different solutions of (3.17) in case $c_1 = 1/3$.

where

$$G_1 = \exp(\sqrt{Z}) = \xi(Z) + \sqrt{Z}\eta_0(Z) \tag{3.19}$$

and

$$G_2 = \exp(\mathrm{i}\sqrt{-Z}) = \xi(Z) + \mathrm{i}\sqrt{-Z}\eta_0(Z). \tag{3.20}$$

For very small values of $|Z|$ we also have

$$c_2 = 1 + \frac{1}{135}Z + \frac{19}{102060}Z^2 + \mathcal{O}(Z^3)$$

showing that, in the limit of $\omega \to 0$, the value of c_2 tends to the classical value of the RadauIIA method. Introducing this expression for c_2 into (3.10) and (3.16) and considering the Taylor series with respect to Z one obtains

$$b_1 = \frac{3}{4} + \frac{7}{720}Z + \frac{41}{453600}Z^2 + \mathcal{O}(Z^3),$$

$$b_2 = \frac{1}{4} - \frac{7}{720}Z - \frac{41}{453600}Z^2 + \mathcal{O}(Z^3),$$

$$a_{11} = \frac{5}{12} + \frac{119}{6480}Z - \frac{403}{4082400}Z^2 + \mathcal{O}(Z^3),$$

$$a_{12} = -\frac{1}{12} + \frac{41}{6480}Z - \frac{239}{1360800}Z^2 + \mathcal{O}(Z^3),$$

$$a_{21} = \frac{3}{4} + \frac{7}{240}Z + \frac{41}{453600}Z^2 + \mathcal{O}(Z^3),$$

$$a_{22} = \frac{1}{4} - \frac{7}{240}Z - \frac{41}{453600}Z^2 + \mathcal{O}(Z^3).$$

Case 2b ($c_2 = 1$): We now have in (3.17) a transcendental equation in c_1 and a contourplot as in Fig. 2 shows that there are again several solutions; however, we are primarily interested in the

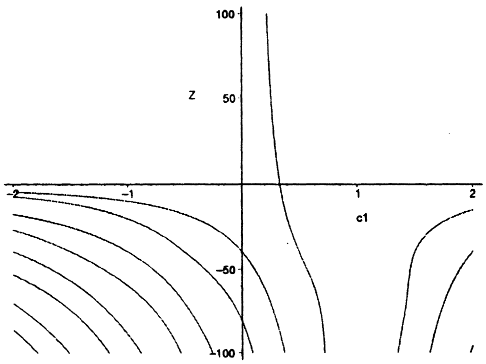

Fig. 2. The different solutions of (3.17) in case $c_2 = 1$.

curve passing through $(c_1, Z) = (1/3, 0)$. For small values of Z, one can solve (3.17) explicitly for c_1 to obtain

$$c_1 = \begin{cases} \dfrac{1}{\sqrt{z}} \log\left(\dfrac{-G_1 + 1 + \sqrt{Z}G_1}{-1 + G_1 - \sqrt{Z}}\right), & Z > 0 \\ \dfrac{1}{3}, & Z = 0, \\ -\dfrac{\mathrm{i}}{\sqrt{-Z}} \log\left(\dfrac{-G_2 + 1 + \mathrm{i}\sqrt{-Z}G_2}{-1 + G_2 - \mathrm{i}\sqrt{-Z}}\right), & Z < 0. \end{cases} \tag{3.21}$$

A series expansion gives

$$c_1 = \frac{1}{3} - \frac{1}{405} Z + \frac{1}{34020} Z^2 + \mathcal{O}(Z^3) \tag{3.22}$$

and introducing this c_1 in (3.16) and (3.10) a Taylor series development with respect to Z gives

$$a_{11} = \frac{5}{12} + \frac{11}{720} Z - \frac{23}{50400} Z^2 + \mathcal{O}(Z^3),$$

$$a_{12} = -\frac{1}{12} + \frac{1}{144} Z - \frac{17}{50400} Z^2 + \mathcal{O}(Z^3),$$

$$a_{21} = b_1 = \frac{3}{4} + \frac{1}{240} Z - \frac{1}{16800} Z^2 + \mathcal{O}(Z^3),$$

$$a_{22} = b_2 = \frac{1}{4} - \frac{1}{240} Z + \frac{1}{16800} Z^2 + \mathcal{O}(Z^3)$$

showing again that this result is a real extension of the (polynomial based) RadauIIA method.

In cases 2a and 2b the final equation integrates exactly the functions 1, x and $\exp(\pm\omega x)$, which are the linear-independent solutions of the differential equation $y^{(4)} - \omega^2 y'' = 0$; on the other hand the internal stages still only integrate the functions $1, \exp(\pm\omega x)$ which are the linear-independent solutions of the linear differential equation $y^{(3)} - \omega^2 y'$. Taking this into account and expression (3.4) the plte should be of the form

$$\mathrm{plte}(\mathrm{RadauIIA}, s = 2, \exp, \mathrm{case}\ 2) = -\frac{h^4}{216}(-\omega^2 y^{(2)} + y^{(4)} - 4 f_y(-\omega^2 y' + y^{(3)})), \tag{3.23}$$

which is exactly the same as in case 1.

3.2.3. Order 4 methods

Case 1 (*Fixed c-Values*): In order to obtain an algebraic order 4 method we introduce $c_1 = (3 - \sqrt{3})/6$ and $c_2 = (3 + \sqrt{3})/6$ into (3.10). Considering the Taylor expansion with respect to Z

one obtains (Gauss, case 1):

$$b_1 = b_2 = \frac{1}{2} + \frac{1}{8640} Z^2 + \mathcal{O}(Z^3),$$

$$a_{11} = \frac{1}{4} + \frac{\sqrt{3}}{288} Z + \frac{3 - 4\sqrt{3}}{51840} Z^2 + \mathcal{O}(Z^3),$$

$$a_{12} = \frac{1}{4} - \frac{1}{6}\sqrt{3} + \frac{\sqrt{3}}{864} Z + \frac{3 - 4\sqrt{3}}{51840} Z^2 + \mathcal{O}(Z^3),$$

$$a_{21} = \frac{1}{4} + \frac{1}{6}\sqrt{3} - \frac{\sqrt{3}}{864} Z + \frac{3 + 4\sqrt{3}}{51840} Z^2 + \mathcal{O}(Z^3),$$

$$a_{22} = \frac{1}{4} - \frac{\sqrt{3}}{288} Z + \frac{3 + 4\sqrt{3}}{51840} Z^2 + \mathcal{O}(Z^3).$$

Here again one can check (by considering the algebraic order conditions in which the ω-dependent coefficients are plugged in) that the order is four and that the plte is given by

$$\begin{aligned} &\text{plte}(\text{Gauss}, s = 2, \exp, \text{case } 1) \\ &= \frac{h^5}{4320}((-\omega^2 y^{(3)} + y^{(5)}) + \omega^2(-\omega^2 y' + y^{(3)}) \\ &\quad -5 f_y(-\omega^2 y^{(2)} + y^{(4)}) + 10(f_y^2 - (f_{xy} + f_{yy} f))(-\omega^2 y' + y^{(3)})). \end{aligned}$$

The first two terms of the last factor can be rewritten as $-\omega^4 y' + y^{(5)}$, which reflects the fact that $b_1 + b_2 = 1 + \mathcal{O}(Z^2)$.

Case 2 (*ω-Dependent c-Values*): We will discuss two cases: one for which $P' = 0$ (case 2a) and one for which $P' = 1$ (case 2b).

Case 2a ($P' = 0$): We take $P' = 0$ such that $K' = 2$ and solve Eqs. (3.6)–(3.7), (3.15) and

$$L_2(h, \mathbf{b}) = h^2 \left(b_1 c_1 + b_2 c_2 - \frac{1}{2} \right) = 0. \tag{3.24}$$

Eqs. (3.15) and (3.24) give simple expressions for b_1 and b_2 in terms of the knot points, i.e.,

$$b_1 = \frac{1 - 2c_2}{2(c_1 - c_2)}, \quad b_2 = \frac{2c_1 - 1}{2(c_1 - c_2)}.$$

Due to symmetry reasons we can hope for a solution if $c_2 = 1 - c_1$, such that $b_1 = b_2 = 1/2$. For this choice the system of nonlinear equations considered has a solution, a fact which has been confirmed by [9] in his study of Gauss quadrature rules for oscillatory functions. Introducing the new variable $d > 0$ as $d = \frac{1}{2} - c_1 = c_2 - \frac{1}{2}$, the resulting condition can be written as

$$\xi(d^2 Z) - \eta_0(Z/4) = 0. \tag{3.25}$$

This equation can be solved for d as a function of Z. The graph of the solution is given in Fig. 3.

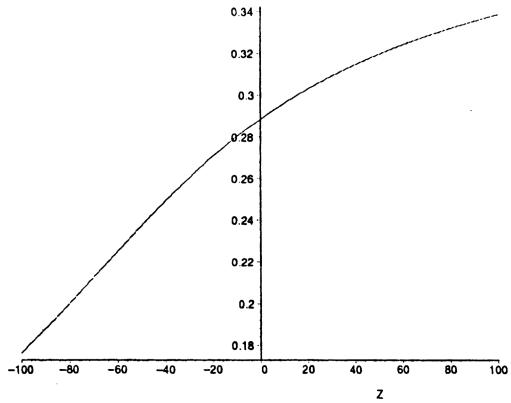

Fig. 3. A plot of the solution d of (3.25) as a function of Z.

The solution for c_2 can then be written as

$$c_2 = \begin{cases} \dfrac{1}{\sqrt{Z}} \log\left(\dfrac{G_1 - 1 + \sqrt{(G_1-1)^2 - ZG_1}}{\sqrt{Z}} \right), & Z > 0, \\ \dfrac{3+\sqrt{3}}{6}, & Z = 0, \\ \dfrac{1}{i\sqrt{-Z}} \log\left(\dfrac{G_2 - 1 + \sqrt{(G_2-1)^2 - ZG_2}}{i\sqrt{-Z}} \right), & Z < 0 \end{cases} \tag{3.26}$$

with G_1 and G_2, respectively, defined in (3.19)–(3.20). A series expansion gives

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6} - \frac{\sqrt{3}}{2160} Z + \frac{\sqrt{3}}{403200} Z^2 + \mathcal{O}(Z^3),$$

$$c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6} + \frac{\sqrt{3}}{2160} Z - \frac{\sqrt{3}}{403200} Z^2 + \mathcal{O}(Z^3)$$

and

$$a_{11} = \frac{1}{4} + \frac{\sqrt{3}}{360} Z - \frac{19\sqrt{3}}{302400} Z^2 + \mathcal{O}(Z^3),$$

$$a_{12} = \frac{1}{4} - \frac{1}{6}\sqrt{3} + \frac{\sqrt{3}}{720} Z - \frac{61\sqrt{3}}{1209600} Z^2 + \mathcal{O}(Z^3),$$

$$a_{21} = \frac{1}{4} + \frac{1}{6}\sqrt{3} - \frac{\sqrt{3}}{720} Z + \frac{61\sqrt{3}}{1209600} Z^2 + \mathcal{O}(Z^3),$$

$$a_{22} = \frac{1}{4} - \frac{\sqrt{3}}{360} Z + \frac{19\sqrt{3}}{302400} Z^2 + \mathcal{O}(Z^3).$$

Again these results demonstrate the ω-dependence of (some of) the coefficients of the Butcher tableau and the fact that, as $\omega \to 0$, the classical c_i- and a_{ij}-values are recovered.

The final stage in case 2a integrates exactly the functions $1, x, x^2$ and $\exp(\pm\omega x)$, which are the linear-independent solutions of the differential equation $y^{(5)} - \omega^2 y^{(3)} = 0$; again we have to realize that the internal stages only integrate the functions $1, \exp(\pm\omega x)$ which are linear-independent solutions of $y^{(3)} - \omega y'$ but also of $y^{(4)} - \omega^2 y^{(2)}$.

Taking this into account and form (3.5) the plte should be

$$\begin{aligned}
&\mathrm{plte}(\mathrm{Gauss}, s=2, \exp, \mathrm{case\ 2a})\\
&\quad = \frac{h^5}{4320}(-\omega^2 y^{(3)} + y^{(5)} - 5 f_y(-\omega^2 y^{(2)} + y^{(4)})\\
&\qquad + 10(f_y^2 - (f_{xy} + f_{yy} f))(-\omega^2 y' + y^{(3)})),
\end{aligned}$$

which is the same as in case 1.

Case 2b ($P'=1$): Secondly we consider the choice where $K'=0$ and $P'=1$, i.e., the full exponential fitting case. This means that in order to determine the b_i and c_i-values we combine Eqs. (3.6)–(3.7) with $G^{\pm(1)}(Z, \mathbf{b}) = 0$, which taking into account the properties (1.4) of the ξ and η functions read

$$G^{+(1)}(Z, \mathbf{b}) = \eta_0(Z) - \sum_{i=1}^{2} b_i c_i \eta_0(c_i^2 Z) - \sum_{i=1}^{2} b_i c_i \xi(c_i^2 Z) = 0,$$

$$G^{-(1)}(Z, \mathbf{b}) = -\eta_0(Z) + \xi(Z) - Z \sum_{i=1}^{2} b_i c_i^2 \eta_0(c_i^2 Z) = 0.$$

The solution of these four equations cannot anymore be given in a closed form as it was the case for the other cases studied so far. It is, however, evident that again a solution can only be found provided the c_i-values are ω-dependent. The following results have been obtained in a series expansion form

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6} - \frac{\sqrt{3}}{1080} Z - \frac{13\sqrt{3}}{2721600} Z^2 + \mathcal{O}(Z^3),$$

$$c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6} + \frac{\sqrt{3}}{1080} Z + \frac{13\sqrt{3}}{2721600} Z^2 + \mathcal{O}(Z^3),$$

$$b_1 = \frac{1}{2} - \frac{1}{8640} Z^2 + \mathcal{O}(Z^3),$$

$$b_2 = \frac{1}{2} - \frac{1}{8640} Z^2 + \mathcal{O}(Z^3),$$

$$a_{11} = \frac{1}{4} + \frac{\sqrt{3}}{480} Z - \frac{37\sqrt{3} + 35}{604800} Z^2 + \mathcal{O}(Z^3),$$

$$a_{12} = \frac{1}{4} - \frac{1}{6}\sqrt{3} + \frac{7\sqrt{3}}{4320} Z - \frac{315 + 113\sqrt{3}}{5443200} Z^2 + \mathcal{O}(Z^3),$$

$$a_{21} = \frac{1}{4} + \frac{1}{6}\sqrt{3} - \frac{7\sqrt{3}}{4320}Z + \frac{-315 + 113\sqrt{3}}{5443200}Z^2 + \mathcal{O}(Z^3),$$

$$a_{22} = \frac{1}{4} - \frac{\sqrt{3}}{480}Z + \frac{37\sqrt{3} - 35}{604800}Z^2 + \mathcal{O}(Z^3).$$

The expression for the plte can now be derived as follows. The final stage integrates exactly the functions $1, \exp(\pm\omega x), x\exp(\pm\omega x)$ which are linear-independent solutions of the differential equation $y^{(5)} - 2\omega^2 y^{(3)} + \omega^4 y' = 0$; On the other hand the internal stages still only integrate the functions $1, \exp(\pm\omega x)$ which are the linear-independent solutions of the linear differential equations $y^{(3)} - \omega^2 y' = 0$ and $y^{(4)} - \omega^2 y'' = 0$.

This means that the plte should be of the form:

$$\begin{aligned}&\text{plte(Gauss}, s = 2, \exp, \text{case 2b})\\ &\quad = \frac{h^5}{4320}[\omega^4 y' - 2\omega^2 y^{(3)} + y^{(5)} - 5f_y(-\omega^2 y'' + y^{(4)})\\ &\qquad + 10(f_y^2 - (f_{xy} + f_{yy}f))(-\omega^2 y' + y^{(3)})].\end{aligned}$$

4. Numerical examples

As a first example we consider the problem

$$y' = y, \quad y(0) = 1 \tag{4.1}$$

and we will apply several versions of the RadauIIA method to this problem with fixed stepsize. The stepsizes used are given in the first column of Table 1. In the other columns the absolute values of the global errors in $x = 1$ are given.

First of all, the classical method is applied. In column two of Table 1, we can deduce that this classical method indeed behaves like a third-order method, since halving the stepsize means that the total error is reduced by a factor which is approximately 8.

Secondly, we apply the exponential fitted method (case 1) where $c_1 = 1/3$ and $c_2 = 1$. The value of ω in each step is obtained by annihilating the leading term in the local truncation error as

Table 1
Absolute values of global errors in $x = 1$ of several versions of the RadauIIA method applied to (4.1)

h	Classical	Case 1	Case 2a	Case 2b
1	$5.16\cdot10^{-2}$	$1.33\cdot10^{-15}$	0.00	$1.78\cdot10^{-15}$
$\frac{1}{2}$	$5.55\cdot10^{-2}$	$4.44\cdot10^{-16}$	$8.88\cdot10^{-16}$	$3.11\cdot10^{-15}$
$\frac{1}{4}$	$6.33\cdot10^{-4}$	$8.88\cdot10^{-16}$	$1.78\cdot10^{-15}$	$1.69\cdot10^{-14}$
$\frac{1}{8}$	$7.63\cdot10^{-5}$	0.00	$4.44\cdot10^{-16}$	0.00
$\frac{1}{16}$	$9.37\cdot10^{-6}$	$1.33\cdot10^{-15}$	$1.33\cdot10^{-15}$	$4.44\cdot10^{-16}$

Table 2
Absolute values of the global errors in $x = 1$ of several versions of the RadauIIA method applied to (4.2)

h	Classical	Case 1	Case 2a	Case 2b
1	$8.25\cdot 10^{-2}$	0.00	$3.98\cdot 10^{-3}$	$4.59\cdot 10^{-3}$
	$2.60\cdot 10^{-2}$	$1.11\cdot 10^{-16}$	$9.97\cdot 10^{-3}$	$3.07\cdot 10^{-3}$
$\frac{1}{2}$	$8.91\cdot 10^{-3}$	$1.11\cdot 10^{-16}$	$2.57\cdot 10^{-4}$	$1.12\cdot 10^{-4}$
	$1.83\cdot 10^{-3}$	$1.11\cdot 10^{-16}$	$1.00\cdot 10^{-3}$	$6.61\cdot 10^{-4}$
$\frac{1}{4}$	$1.11\cdot 10^{-3}$	$2.22\cdot 10^{-16}$	$2.48\cdot 10^{-5}$	$5.76\cdot 10^{-6}$
	$2.08\cdot 10^{-1}$	0.00	$1.21\cdot 10^{-4}$	$9.82\cdot 10^{-5}$
$\frac{1}{8}$	$1.40\cdot 10^{-4}$	0.00	$2.77\cdot 10^{-6}$	$1.69\cdot 10^{-6}$
	$2.57\cdot 10^{-5}$	$1.11\cdot 10^{-16}$	$1.50\cdot 10^{-5}$	$1.33\cdot 10^{-5}$
$\frac{1}{16}$	$1.77\cdot 10^{-5}$	$1.11\cdot 10^{-16}$	$3.29\cdot 10^{-7}$	$2.65\cdot 10^{-7}$
	$3.24\cdot 10^{-6}$	$1.11\cdot 10^{-16}$	$1.83\cdot 10^{-6}$	$1.73\cdot 10^{-6}$

computed in (3.14). For this problem we obtain the constant value $\omega=1$. Since the analytical solution $y(x) = \exp(x)$ is in the space of functions which are integrated exactly with that choice for ω, we obtain in column 3 of Table 1 machine accuracy for all values of h.

This is also the case for the exponential fitted method where the $c_1 = 1/3$ and c_2 is determined by (3.18) (case 2a) and for case 2b where $c_2 = 1$ and c_1 is given by (3.21). Indeed, for both methods the constant value $\omega = 1$ is obtained in each step if the leading term in the local truncation error is set equal to zero.

So from Table 1 we conclude that our experimental results agree with the theory.

As a second example, we consider the problem

$$y_1' = -y_2 + \cos x + \sin 2x, \qquad y_1(0) = 0,$$

$$y_2' = y_1 + 2\cos 2x - \sin x, \qquad y_2(0) = 0. \tag{4.2}$$

Its solution is given by

$$y_1(x) = \sin x,$$

$$y_2(x) = \sin 2x.$$

We apply the same methods and again we compare the global errors (for each of the components) at the endpoint. However, since we now have a system of equations, the expressions for the local truncation errors should be interpreted appropriately: f_y is now the Jacobian and for the exponential fitted versions, ω^2 is a diagonal matrix with diagonal elements ω_1^2 and ω_2^2 where ω_1 is the frequency to which the first equation is fitted and ω_2 the one to which the second equation is fitted. To annihilate the leading term of the local truncation error we now solve a system and we obtain $\omega_1^2=-1$, $\omega_2^2=-4$ for all of the three exponential fitted methods, such that we fit to linear combinations of $\sin x$ and $\cos x$ for the first equation and $\sin 2x$ and $\cos 2x$ for the second equation.

The results in Table 2 for the classical method and the exponential fitted method with fixed collocation points (case 1) again confirm the theoretical results. However, the exponential fitted methods where one of the c's is ω-dependent (cases 2a and 2b) do not integrate the system exactly. Although in each case the plte was annihilated, these methods still behave like third-order methods.

This at first sight surprising result shows that there is a great distinction between methods with fixed collocation points and methods with ω-dependent collocation points. The analysis of this discrepancy will be discussed in the next section.

5. Fixed versus ω-dependent knot points

There are several ways in which an exponential fitted method can be applied to a system of equations. A first approach is to use the same ω to fit to all the components of the systems. This approach may be well suited if all components exhibit the same behaviour, but if serious differences arise between components it is not possible to determine a value for ω for which the error in all components will be reduced significantly compared to the classical case. In that case a better approach is to use a separate ω for each component such that the EFRK method becomes a partitioned method [6].

A partitioned method can be applied to a system of the form

$$\begin{aligned} y' &= f(x, y, z), \\ z' &= g(x, y, z), \end{aligned} \tag{5.1}$$

where y and z can be vectors of different dimensions. The idea of a partitioned RK method is to treat the y-variables with one RK method and the z-variables with a second method. This idea can be extended to more than two methods.

It is well known from the theory of partitioned RK methods that, if a partitioned method is made up of two methods of order p, its order cannot exceed p. The order conditions for partitioned RK methods can be divided in two categories: the usual order conditions for RK methods and additional so-called coupling order conditions. It is only when these additional conditions are fulfilled that the partitioned RK method also has order p.

Of course, the different methods which are used in our exponential fitted partitioned method are very similar: they all reduce to the same classical method if all ω's tend to 0. With this in mind, it is easy to verify by considering the different series expansions that for all the 2-stage methods (Lobatto, Radau, Gauss) considered in this paper the order of the partitioned method is the same as the order of the originating RK method.

However, these same series expansions reveal that extra terms may occur in the expressions for the leading term of the local truncation errors of the partitioned RK methods. We obtain the following expressions for the exponential fitted Radau IIA methods when applied to system (5.1) where y and z are scalars.

Case 1:

$$\begin{aligned} &\mathrm{plte}(\mathrm{RadauIIA}, s=2, \exp, \mathrm{case}\ 1) \\ &\quad = -\frac{h^4}{216}\left\{ -\begin{pmatrix} \omega_1^2 & 0 \\ 0 & \omega_2^2 \end{pmatrix}\begin{pmatrix} y^{(2)} \\ z^{(2)} \end{pmatrix} + \begin{pmatrix} y^{(4)} \\ z^{(4)} \end{pmatrix} \right. \\ &\qquad \left. -4\begin{pmatrix} f_y & f_z \\ g_y & g_z \end{pmatrix}\left[-\begin{pmatrix} \omega_1^2 & 0 \\ 0 & \omega_2^2 \end{pmatrix}\begin{pmatrix} y' \\ z' \end{pmatrix} + \begin{pmatrix} y^{(3)} \\ z^{(3)} \end{pmatrix} \right] \right\}. \end{aligned}$$

Case 2a:

$$\begin{aligned}
&\text{plte}(\text{RadauIIA}, s=2, \exp, \text{case 2a})\\
&= -\frac{h^4}{216}\left\{-\begin{pmatrix}\omega_1^2 & 0\\ 0 & \omega_2^2\end{pmatrix}\begin{pmatrix}y^{(2)}\\ z^{(2)}\end{pmatrix}+\begin{pmatrix}y^{(4)}\\ z^{(4)}\end{pmatrix}\right.\\
&\quad -4\begin{pmatrix}f_y & f_z\\ g_y & g_z\end{pmatrix}\left[-\begin{pmatrix}\omega_1^2 & 0\\ 0 & \omega_2^2\end{pmatrix}\begin{pmatrix}y'\\ z'\end{pmatrix}+\begin{pmatrix}y^{(3)}\\ z^{(3)}\end{pmatrix}\right]\\
&\quad \left.-\frac{2}{5}\begin{pmatrix}(\omega_1^2-\omega_2^2)f_z g\\ (\omega_2^2-\omega_1^2)g_y f\end{pmatrix}\right\}.
\end{aligned}$$

Case 2b:

$$\begin{aligned}
&\text{plte}(\text{RadauIIA}, s=2, \exp, \text{case 2b})\\
&= -\frac{h^4}{216}\left\{-\begin{pmatrix}\omega_1^2 & 0\\ 0 & \omega_2^2\end{pmatrix}\begin{pmatrix}y^{(2)}\\ z^{(2)}\end{pmatrix}+\begin{pmatrix}y^{(4)}\\ z^{(4)}\end{pmatrix}\right.\\
&\quad -4\begin{pmatrix}f_y & f_z\\ g_y & g_z\end{pmatrix}\left[-\begin{pmatrix}\omega_1^2 & 0\\ 0 & \omega_2^2\end{pmatrix}\begin{pmatrix}y'\\ z'\end{pmatrix}+\begin{pmatrix}y^{(3)}\\ z^{(3)}\end{pmatrix}\right]\\
&\quad \left.+\frac{2}{5}\begin{pmatrix}(\omega_1^2-\omega_2^2)f_z g\\ (\omega_2^2-\omega_1^2)g_y f\end{pmatrix}\right\}.
\end{aligned}$$

In case 1, it turns out that there are no extra terms. The values for $\omega_1^2=-1$ and $\omega_2^2=-4$ which annihilate the leading term were already correctly computed and since they are also the squares of the frequencies of the components of the exact solution of the problem, we have machine accuracy.

For the cases 2a and 2b there are extra terms, such that the true values of ω_1^2 and ω_2^2 which make the plte vanish do not coincide with -1 and -4. In fact, these true values are given by

Case 2a:

$$\begin{aligned}
\omega_1^2 &= -\frac{128\sin^3 x+220\sin^2 x-63\sin x-120}{32\sin^3 x+172\sin^2 x-15\sin x-96},\\
\omega_2^2 &= -\frac{128\sin^3 x+640\sin^2 x-63\sin x-360}{32\sin^3 x+172\sin^2 x-15\sin x-96}.
\end{aligned}\tag{5.2}$$

Case 2b:

$$\begin{aligned}
\omega_1^2 &= -\frac{128\sin^3 x-60\sin^2 x-63\sin x+40}{32\sin^3 x-108\sin^2 x-15\sin x+64},\\
\omega_2^2 &= -\frac{128\sin^3 x-480\sin^2 x-63\sin x+280}{32\sin^3 x-108\sin^2 x-15\sin x+64}.
\end{aligned}\tag{5.3}$$

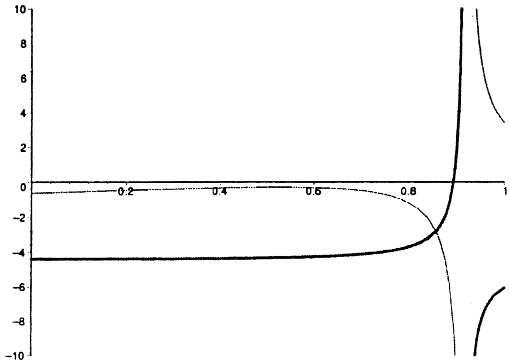

Fig. 4. The values for ω_1^2 (thin line) and ω_2^2 (thick line) for case 2b applied to problem (4.2).

Table 3
Absolute values of the global errors in $x = 1$ of the ω-dependent RadauIIA methods applied to (4.2). The values for ω are obtained from (5.2)–(5.3)

h	Case 2a	Case 2b
1	$7.11{\cdot}10^{-3}$	$4.06{\cdot}10^{-4}$
	$1.71{\cdot}10^{-4}$	$8.30{\cdot}10^{-3}$
$\frac{1}{2}$	$3.53{\cdot}10^{-4}$	$1.02{\cdot}10^{-4}$
	$5.07{\cdot}10^{-5}$	$3.93{\cdot}10^{-4}$
$\frac{1}{4}$	$2.91{\cdot}10^{-5}$	$1.72{\cdot}10^{-5}$
	$7.92{\cdot}10^{-6}$	$1.78{\cdot}10^{-5}$
$\frac{1}{8}$	$4.45{\cdot}10^{-7}$	$3.00{\cdot}10^{-6}$
	$2.88{\cdot}10^{-7}$	$3.35{\cdot}10^{-7}$
$\frac{1}{16}$	$8.73{\cdot}10^{-8}$	$4.64{\cdot}10^{-8}$
	$4.01{\cdot}10^{-8}$	$9.64{\cdot}10^{-8}$

In Fig. 4 the values for ω_1^2 and ω_2^2 are plotted for case 2b (case 2a is very similar). The optimal values for ω_1 and ω_2 are no longer constants, but rather defined by a x-dependent periodic function. One notices that, already at the start of the integration interval, these computed values are rather big corrections to the true frequencies of the components of the solution. As the integration advances the computed ω values even move further away (ω_2^2 even becomes positive such that we fit the second component to hyperbolic functions rather than trigonometric functions) and for $x \approx 0.917$ there is a discontinuity.

Since the computed values for the ω's do not coincide with the squares of the frequencies in the solutions, we can no longer hope for machine accuracy: we can only obtain a raise of the order of the partitioned method from 3 to 4. This is indeed what we find in Table 3 and in Fig. 5. In Table 3 we show the absolute values of the errors in the endpoint $x = 1$ for different values of h. The upper line each time corresponds to the first component, the lowest line to the second component. In Fig. 5

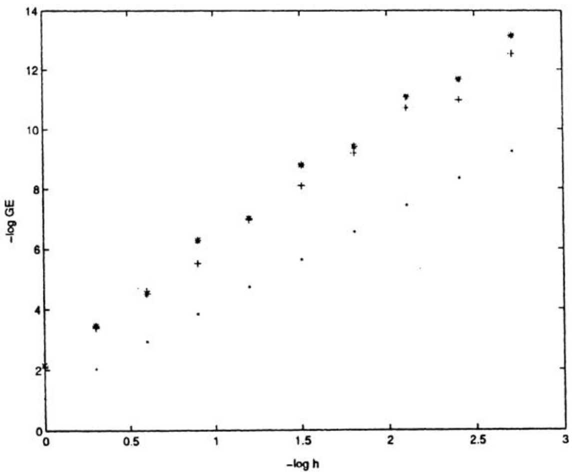

Fig. 5. A log–log plot (base 10) of the step size versus the global error in the endpoint for the classical RadauIIA method (dots) and its exponential fitted cases IIA (stars) and IIB (crosses).

we display $-\log_{10} h$ versus $-\log_{10}$GE where GE is the global error (in the Euclidean norm) in the endpoint. We notice that, for the exponential fitted methods, the points slightly deviate from a straight line. This is mainly due to the discontinuity in the expressions which determine the ω's. However, if we compute the slopes of the best fitting straight lines we obtain 3.009 for the classical RadauIIA method, while we have 4.040 for the EFRK 2a case and 3.823 for the EFRK 2b case. Clearly, these numbers confirm the raise of the order.

6. Conclusion

In this paper, we have constructed several exponential fitted versions of well-known 2-stage RK methods. These EFRK methods can be divided in two classes: methods for which all of the c-points are fixed constants (case 1) and methods for which some of the c-points are frequency dependent (case 2). From a theoretical point of view, both classes of methods are quite easy to construct. However, in practice, there is a big difference. Although there exist problems for which both kinds of methods give machine accuracy, there also exist problems for which machine accuracy is obtained for case 1 but not for case 2. The converse is never the case. A closer examination of the local truncation error also revealed that, unlike the methods of case 1, the methods of case 2 behave like partitioned EFRK methods. In that case, an accurate computation of the frequencies of the different components of the solution by annihilating the plte is no longer possible due to presence of extra coupling terms. Therefore, for solving systems of equations the methods with fixed knot points should be preferred above the methods with variable knot points. In the special case of scalar problems, both kinds of methods can be applied. This special case (and in particular the quadrature problem) will be discussed in a separate paper.

Appendix A.

The functions $\xi(Z), \eta_0(Z), \eta_1(Z), \ldots,$ were originally introduced in [7, Section 3.4] and denoted there as $\bar{\xi}(Z), \bar{\eta}_0(Z), \bar{\eta}_1(Z), \ldots$.

They are defined as follows. The functions $\xi(Z)$ and $\eta_0(Z)$ are generated first by the formulae

$$\xi(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z < 0, \\ \cosh(Z^{1/2}) & \text{if } Z \geqslant 0, \end{cases}$$

$$\eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0, \\ 1 & \text{if } Z = 0, \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0, \end{cases}$$

while $\eta_s(Z)$ with $s > 0$ are further generated by recurrence

$$\eta_1(Z) = [\xi(Z) - \eta_0(Z)]/Z,$$

$$\eta_s(Z) = [\eta_{s-2}(Z) - (2s-1)\eta_{s-1}(Z)]/Z, \quad s = 2, 3, 4, \ldots$$

if $Z \neq 0$ and by following values at $Z = 0$:

$$\eta_s(0) = 1/(2s+1)!!, \quad s = 1, 2, 3, 4, \ldots \ .$$

These functions satisfy the following differentiation property with respect to Z:

$$\xi'(Z) = \frac{1}{2}\eta_0(Z) \quad \text{and} \quad \eta_s'(Z) = \frac{1}{2}\eta_{s+1}(Z), \qquad s = 0, 1, 2, \ldots \ . \tag{A.1}$$

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