User-friendly expressions of the coefficients of some exponentially fitted methods^{*}

Dajana Conte¹, Raffaele D'Ambrosio², Giuseppe Giordano¹, L. Gr. Ixaru^{3,4}, and Beatrice Paternoster¹

¹ Department of Mathematics, University of Salerno, Fisciano, Salerno, Italy dajconte@unisa.it,gigiordano@unisa.it,beapat@unisa.it

² Department of Information Engineering and Computer Science and Mathematics, University of L'Aquila raffaele.dambrosio@univaq.it

 $^3\,$ Horia Hulubei National institute of Physics and Nuclear Engineering - Bucharest, Romania

⁴ Academy of Romanian Scientists, 54 Splaiul Independenţei, 050094, Bucharest, Romania ixaru@theory.nipne.ro

Abstract. The purpose of this work consists in reformulating the coefficients of some exponentially-fitted (EF) methods with the aim of avoiding numerical cancellations and loss of precision. Usually the coefficients of an EF method are expressed in terms of $\nu = \omega h$, where ω is the frequency and h is the step size. Often, these coefficients exhibit a 0/0 indeterminate form when $\nu \to 0$. To avoid this feature we will use two sets of functions, called C and S, which have been introduced by Ixaru in [62]. We show that the reformulation of the coefficients in terms of these functions leads to a complete removal of the indeterminacy and thus the convergence of the corresponding EF method is restored. Numerical results will be shown to highlight these properties.

Keywords: Exponential fitting, C and S sets of functions, η_m set of functions

1 Introduction

Exponential fitting is a mathematical procedure to generate numerical methods for different problems with a pronounced oscillatory or hyperbolic behaviour, usualy occurring in interpolation, numerical differentiation and quadrature [30, 31, 33, 35, 72, 61, 65, 66, 80], numerical solution of first order ordinary differential equations [4, 3, 27, 40, 43, 50, 61, 70, 74, 75, 77, 78, 81], second order differential equations [55, 64], integral equations [15, 16], fractional differential equations [1], partial differential equations [14, 45, 46, 51, 53]. This procedure has been introduced in [63]. Its central idea consists in determining the coefficients of a

^{*} The authors Conte, D'Ambrosio, Giordano and Paternoster are members of the GNCS group. This work is supported by GNCS-INDAM project and by PRIN2017-MIUR project.

numerical method by asking that the method is exact for the following set of functions, which is called a *fitting space*:

$$\mathcal{F} = \{1, x, \dots, x^{K}, e^{\pm \mu x}, x e^{\pm \mu x}, \dots, x^{P} e^{\pm \mu x}\}$$
(1)

where μ may be real or imaginary. The coefficients are functions of the parameter $\nu = \omega h$, where ω is the frequency of the oscillatory or hyperbolic functions and h is the step size. The values of μ to be used in (1) are the imaginary $\mu = i\omega$ and real $\mu = \omega$, respectively.

Often, these coefficients exhibit the indeterminate form 0/0 when $\nu \to 0$ such that, in order to restore the convergence of the corresponding numerical methods when ν is small (in practice this depends on how small is the step size h), it is necessary to make use of the Taylor series of the coefficients. Expressed in different words, an accurate computation of the EF coefficients requires the knowledge of four different formulas (an analytic formula valid for big ν and a power series for small ν , for each of the trigonometrical or hyperbolic fitting).

In the paper [62] a method was described to replace the four formulas by a single one. The coefficients have been expressed in terms of two sets of particular functions, called C(Z) and S(Z), where $Z = \pm \nu^2$, for real and imaginary μ . A similar method has been introduced in the paper [30], in which the coefficients are expressed in terms of $\eta_m(Z)$ functions.

The work is organized as follows. In Section 2 we recall the two sets of C and S functions, and in Section 3 the general procedure for the conversion of the coefficient in terms of C and S functions is briefly presented. In Section 4 we reformulate the coefficients for the methods in [69, 71]. In Section 5 numerical experiments are presented to show how the converted coefficients restore the convergence of the method.

2 C and S functions

The original $\nu = \mu h$ is replaced by the new $Z = \nu^2$ which is negative if ν is imaginary and positive when ν is real. Thus, Z < 0 and Z > 0 cover the trigonometric and hyperbolic case, respectively.

To define the sets of functions C and S we rely on the family of functions $\eta_m(Z)$ functions, $m = -1, 0, 1, \dots, \dots$:

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

and, for $Z \neq 0$,

$$\eta_m(Z) = [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z, \ m = 1, 2, 3, \dots$$
(3)

while for Z = 0,

$$\eta_m(0) = 1/(2m+1)!!, \ m = 1, 2, 3, \dots$$
(4)

The two sets of C and S functions are defined as follows: $C_{-1}(Z)$ and $S_{-1}(Z)$ are given by the first two η functions,

$$C_{-1}(Z) = \eta_{-1}(Z), S_{-1}(Z) = \eta_0(Z)$$
(5)

while the next ones are derived by recurrence for $Z \neq 0$,

$$C_n(Z) = \frac{C_{n-1}(Z) - C_{n-1}(0)}{Z}, S_n(Z) = \frac{S_{n-1}(Z) - S_{n-1}(0)}{Z}, \text{ for } n = 0, 1, 2, \dots,$$
(6)

and by the following values at Z = 0,

$$C_n(0) = \frac{1}{(2n+2)!}, S_n(0) = \frac{1}{(2n+3)!},$$
for any $n = 0, 1, 2, \dots$ (7)

An important property is the reverse relations:

$$C_n(Z) = ZC_{n+1}(Z) + C_n(0), S_n(Z) = ZS_{n+1} + S_n(0).$$
(8)

for n = -1, 0, 1, ... For an accurate computation of these functions, it is necessary to introduce their series expansions:

$$C_n(Z) = \sum_{k=0} \frac{Z^k}{[2(k+n+1)]!}, S_n(Z) = \sum_{k=0} \frac{Z^k}{[2(k+n)+3]!}.$$
 (9)

Note: We acknowledge with thanks a recent private communication by Prof. Ander Murua that sets C and S are directly related to the Stumpff functions $c_n(Z)(n = 0, 1, 2, 3, ..)$:

$$C_n(Z) = c_{2n+2}(-Z), \ S_n(Z) = c_{2n+3}(-Z).$$

For the Stumpff functions see [83] and references therein.

3 Procedure for the conversion of coefficients

Now we describe the procedure introduced in [62] for the conversation of the coefficients. Let $\sigma(z)$, a generic coefficient derived by EF technique:

$$\sigma\left(z\right) = \frac{\overline{N}\left(z\right)}{\overline{D}\left(z\right)}$$

where $\overline{N}(z)$ and $\overline{D}(z)$ contains trigonometrical or hyperbolic functions and tend to 0 when $z \to 0$.

Let us denote generically by \overline{F} any of numerator \overline{N} or denominator \overline{D} , and treated separately these two functions. The procedure has two steps. In the first step, $\overline{F}(z)$ is expressed in terms of Z in the following way:

$$\overline{F}(z) = z^k F(Z) \tag{10}$$

where k = 0, 1 and

$$F(Z) = \sum_{m=0}^{M} Z^{m} F_{m}(Z) .$$
(11)

The second step consists in factorizing Z in F(Z) as many times as possible until the form

$$F(Z) = Z^m F^*(Z) \tag{12}$$

where $m \ge 0$ and $F^*(Z) \ne 0$.

To be able to factorize Z in F(Z), we have to first evaluate $F_0(Z)$ at Z = 0. If $F_0(0) \neq 0$, then no Z factorization is possible and the procedure is stopped. Instead, if $F_0(0) = 0$, then

$$\mathcal{F}(Z) = F_0(Z) = Z \Delta F_0(Z),$$

take m = 1 and the following algorithmic applies:

- 1. Form $\mathcal{F}_m(Z) = \Delta F_{m-1}(Z) + F_m(Z)$ and evaluate in 0; 2. If $\mathcal{F}_m(0) = 0$, one factorization of Z is possible and we put $\mathcal{F}_m(Z) =$ $Z\Delta F_m(Z)$, then determine $\Delta F_m(Z)$, increase m by 1, and go to (1);
- 3. If $\mathcal{F}_m(0) \neq 0$, the procedure is stopped and

$$F(Z) = Z^m F^*(Zz) \tag{13}$$

where,

$$F^{*}(Z) = \begin{cases} \Delta F_{m-1}(Z) + \sum_{i=0}^{M-m} Z^{i} F_{m+i} & \text{if } m \leq M, \\ \Delta F_{m-1}(Z) & \text{if } m > M \end{cases}$$
(14)

In the most cases, \mathcal{F}_m is a linear combination of terms containing functions from sets C and S:

$$\mathcal{F}_m(Z) = K + \sum_{j \ge -1} \left[a_j C_j(\alpha_j Z) + b_j S_j(\beta_j Z) \right]$$
(15)

where a_j, b_j, K are constant, and $\alpha_j, \beta_j \ge 0$. By replacing (8) in (15), the following expression is obtained:

$$\mathcal{F}_m(Z) = \mathcal{F}_m(0) + Z \sum_{j \ge -1} \left[a_j \alpha_j C_{j+1}(\alpha_j Z) + b_j \beta_j S_{j+1}(\beta_j Z) \right].$$
(16)

If $\mathcal{F}_m(0) = 0$, then the expression of $\Delta_m(Z)$ is thus obtained:

$$\Delta F_m(Z) = \sum_{j \ge -1} \left[a_j \alpha_j C_{j+1}(\alpha_j Z) + b_j \beta_j S_{j+1}(\beta_j Z) \right].$$
(17)

After applying the procedure described for the numerator and the denominator of the coefficient, the **user-friendly** reformulation of the coefficient is obtained:

$$\sigma(Z) = \frac{N^*(Z)}{D^*(Z)},\tag{18}$$

where $N^*(0) \neq 0$ and $D^*(0) \neq 0$.

4 Reformulation of the coefficients

In this Section we reformulate the coefficients of two relevant classes of EF numerical methods [69, 71] in terms of the C and S functions.

Example 1: The first class of methods, developed by Simos et al. in [69] regards the numerical solution of the second-order Initial Value Problems (IVPs) of the form:

$$\begin{cases} y'' = f(x, y(x)) \\ y(x_0) = y_0 \\ y'(x_0) = y'_0 \end{cases}$$
(19)

The scheme examined in [69] is of the form:

$$y_{n+1} + d_0 y_n + d_1 y_{n-1} + d_2 y_{n-2} + d_1 y_{n-3} + d_0 y_{n-4} + y_{n-5} = h^2 \left(\tilde{d}_0 \tilde{y}_{n+1}'' + \tilde{d}_1 y_n'' + \tilde{d}_2 y_{n-1}'' + \tilde{d}_3 y_{n-2}'' + \tilde{d}_2 y_{n-3} + \tilde{d}_1 y_{n-4} + \tilde{d}_0 y_{n-5}'' \right)$$
(20)

where \tilde{y}_{n+1} is determined by solving

$$\tilde{y}_{n+1} + c_0 y_n + c_1 y_{n-1} + c_2 y_{n-2} + c_1 y_{n-3} + c_0 y_{n-4} + y_{n-5} =
h^2 \left(\tilde{c}_0 y_n'' + \tilde{c}_1 y_{n-1}'' + \tilde{c}_2 y_{n-2}'' + \tilde{c}_1 y_{n-3}'' + \tilde{c}_0 y_{n-4}'' \right).$$
(21)

and using $\tilde{y}_{n+1}'' = f(x_{n+1}, \tilde{y}_{n+1})$ in (20).

The classical version has the constant coefficients:

$$\tilde{c}_0^{\text{class}} = \frac{51484823}{17645880}, \tilde{c}_1^{\text{class}} = \frac{23362512}{735245}, \tilde{c}_2^{\text{class}} = -\frac{723342859}{8822940} \tag{22}$$

$$c_{0} = \frac{12519323}{504168}, c_{1} = \frac{2712635}{63021}, c_{2} = -\frac{551}{4}$$

$$d_{0} = -\frac{23362512}{735245}, d_{1} = \frac{84437}{105035}, d_{2} = -\frac{9}{5} \qquad (23)$$

$$\tilde{d}_{0} = \frac{1}{15}, \tilde{d}_{1} = \frac{209837}{210070}, \tilde{d}_{2} = \frac{320221}{315105}, \tilde{d}_{3} = \frac{638003}{315105}$$

see [57].

In [69] the exponential fitting procedure is applied to produce the following ν dependent expressions for the \tilde{c} coefficients :

$$\begin{split} \tilde{c}_{0}^{\text{ef}} &= -\frac{1}{2016672\nu^{6}\sin^{3}(\nu)} \Big(3(4965191\nu^{4} - 82890689\nu^{2} + 22589400)\sin(\nu) \\ &- 48(69329\nu^{2} - 308970)\sin(2\nu) - (4965191\nu^{4} - 8059857\nu^{2} - 68357160)\sin(3\nu) \\ &+ 7562520(3\nu^{2} - 10)\sin(4\nu) - (59935259\nu^{2} - 95582232)\nu\cos(\nu) \\ &- 32(437993\nu^{2} + 2928636)\nu\cos(2\nu) - 3(4965191\nu^{2} + 13671432)\nu\cos(3\nu) \\ &+ 75625200\nu\cos(4\nu) + 48(875986\nu^{2} - 759933)\nu \Big), \end{split}$$

$$\begin{split} \tilde{c}_{1}^{\text{eff}} &= \frac{1}{1008336\nu^{6} \sin^{3}(\nu)} \left(-24(875986\nu^{4} + 231349\nu^{2} - 617940) \sin(\nu) \right. \\ &\quad -18(14126869\nu^{2} - 7562520) \sin(2\nu) + 4(1751972\nu^{4} + 9751899\nu^{2} - 15198660) \sin(3\nu) \\ &\quad +3(4965191\nu^{2} + 22785720) \sin(4\nu) + 3781260(3\nu^{2} - 20) \sin(5\nu) \\ &\quad +64(875986\nu^{2} - 2650563)\nu \cos(\nu) - 12(14126869\nu^{2} - 4537512)\nu \cos(2\nu) \\ &\quad -2(4965191\nu^{2} + 13671432)\nu \cos(4\nu) + 60500160\nu \cos(5\nu) \\ &\quad +6(4965191\nu^{2} + 13671432)\nu \right), \end{split}$$

The other coefficients are untouched. They remain the same as in (23). Theoretically we must have

$$\lim_{\nu \to 0} \tilde{c}_i^{\text{ef}} = \tilde{c}_i^{\text{class}} \tag{27}$$

for i = 1, 2, 3, but a direct examination of the EF expressions given in (24-26), shows that these have an indeterminate form 0/0 for $\nu \to 0$ such that, in a numerical approach, a blow up of each coefficient will be obtained when h is decreased (we remind that $\nu = \omega h$).

This is removed by applying the procedure described in the previous Section. Indeed, now we have:

$$\begin{split} \varepsilon_{0}^{\text{CS}} &= \frac{1}{2016672S_{-1}^{3}(Z)} \Big(-59935259C_{2}(Z) - 897009664C_{2}(4Z) - 10858872717C_{2}(9Z) \\ &\quad -95582232C_{3}(Z) + 23991386112C_{3}(4Z) + 269094796056C_{3}(9Z) - 4956173107200C_{3}(16Z) \\ &\quad -14895573S_{1}(Z) + 1206541413S_{1}(9Z) - 248672067S_{2}(Z) - 425957376S_{2}(4Z) \\ &\quad 17626907259S_{2}(9Z) + 371712983040S_{2}(16Z) - 67768200S_{3}(Z) - 7593246720S_{3}(4Z) \\ &\quad -1345473980280S_{3}(9Z) + 19824692428800S_{3}(16Z) \Big); \end{split}$$

The new expressions are also quotients of two ν dependent functions but, as expected, they do no longer exhibit indeterminacy when $\nu \to 0$. Also worth mentioning is that the power of Z in (13) for all these three coefficients is m = 4. The use of η functions has the same effect. In fact, by applying the procedure described in [30], the coefficients expressed by these functions are (see also [23]):

$$\tilde{c}_{0}^{\eta} = \frac{-1071987210\eta_{0}^{4}(Z/64) - 535993605\eta_{0}^{2}(Z/256)(1+\eta_{0}(Z/64)) + \dots}{13552035840(2+Z\eta_{0}^{2}(Z/4) - 2Z\eta_{1}(Z))^{3}}$$
(31)

$$\tilde{c}_{1}^{\eta} = \frac{-2031821820\eta_{0}^{4}(Z/64) - 1015910910\eta_{0}^{2}(Z/256)(1+\eta_{0}(Z/64)) + \dots}{13552035840(2+Z\eta_{0}^{2}(Z/4) - 2Z\eta_{1}(Z))^{3}}$$
(32)

$$\tilde{c}_{2}^{\eta} = \frac{-2146293450\eta_{0}^{4}(Z/64) - 1073146725\eta_{0}^{2}(Z/256)(1+\eta_{0}(Z/64)) + \dots}{6776017920(2+Z\eta_{0}^{2}(Z/4) - 2Z\eta_{1}(Z))^{3}}$$
(33)

The full expressions can be obtained using the Mathematica modules in [30]. Both ways of deriving single formulae, instead of four, are then acceptable, and the expected theoretical behavior

$$\lim_{Z \to 0} \tilde{c}_i^{\text{CS}} = \lim_{Z \to 0} \tilde{c}_i^{\eta} = \tilde{c}_i^{\text{class}},\tag{34}$$

is preserved.

Example 2: We consider the numerical method developed by Ndukum et al. [71] to solve the first-order IVP:

$$\begin{cases} y' = f(x, y(x)) \\ y(a) = y_0 \end{cases}$$

$$(35)$$

with $x \in [a, b]$.

The scheme used is a k-step numerical method of the form:

$$y_{n+k} = \sum_{r=0}^{k-1} \alpha_r(\nu) y_{n+r} + h(\beta_k(\nu) f_{n+k} + \beta_{k+1}(\nu) f_{m+k+1}).$$
(36)

In the paper [71] the authors presented the coefficients of the method corresponding to k = 1, 2, 3, 4, 5. In the paper [62] the case k = 2 has been considered. In the following we consider the case k = 3.

By applying the exponential fitting procedure, the coefficients are [71]:

$$\alpha_0^{\text{ef}} = \frac{5\nu - 11\nu\cos\nu + 7\nu\cos2\nu - \nu\cos3\nu + 4\sin\nu + 2\nu^2\sin\nu - 2\sin2\nu}{7\nu\cos\nu - 17\nu\cos2\nu + 13\nu\cos3\nu - 3\nu\cos4\nu + 4\sin\nu + 2\nu^2\sin2\nu - 2\sin2\nu}$$
(37)

$$\alpha_{1}^{\text{ef}} = \frac{-12\nu + 23\nu\cos\nu - 9\nu\cos2\nu - 3\nu\cos3\nu + \nu\cos4\nu - 2\sin\nu - 6\nu^{2}\sin\nu - 2\sin2\nu + 2\sin3\nu}{7\nu\cos\nu - 17\nu\cos2\nu + 13\nu\cos3\nu - 3\nu\cos4\nu + 4\sin\nu + 2\nu^{2}\sin2\nu - 2\sin2\nu}$$
(38)

$$\alpha_{2}^{\text{ef}} = \frac{7nu - 5\nu\cos\nu - 15\nu\cos2\nu + 17\nu\cos3\nu - 4\nu\cos4\nu + 2\sin\nu + 6\nu^{2}\sin\nu + 2\sin2\nu - 2\sin3\nu}{7\nu\cos\nu - 17\nu\cos2\nu + 13\nu\cos3\nu - 3\nu\cos4\nu + 4\sin\nu + 2\nu^{2}\sin2\nu - 2\sin2\nu}$$
(39)
$$\beta_{3}^{\text{ef}} = \frac{2\nu\cos\nu - 6\nu\cos2\nu + 6\nu\cos3\nu - 2\nu\cos4\nu + 25\sin\nu - 20\sin2\nu + 5\sin3\nu}{7\nu\cos\nu - 17\nu\cos2\nu + 13\nu\cos3\nu - 3\nu\cos4\nu + 4\sin\nu + 2\nu^{2}\sin2\nu - 2\sin2\nu}$$
(40)

$$\beta_4^{\text{ef}} = \frac{-2\nu + 6\nu\cos\nu - 6\nu\cos2\nu + 2\nu\cos3\nu - 13\sin\nu + 12\sin2\nu - 3\sin3\nu}{7\nu\cos\nu - 17\nu\cos2\nu + 13\nu\cos3\nu - 3\nu\cos4\nu + 4\sin\nu + 2\nu^2\sin2\nu - 2\sin2\nu}$$
(41)

which all exhibit the 0/0 indeterminacy. The coefficients modified by means of the the procedure described in the previous Section are:

$$\begin{split} \hat{\alpha}_{0}^{\text{CS}} &= \frac{1 + (6(3C_{2}(Z) - 256C_{2}(4Z) + 1701C_{2}(9Z) - 2048C_{2}(16Z))}{-7C_{2}(Z) + 1088C_{2}(4Z) - 9477C_{2}(9Z) + 12288C_{2}(16Z) + 2S_{1}(Z) - 4S_{2}(Z) + 256S_{2}(4Z)} \end{split} \tag{42} \\ \tilde{\alpha}_{1}^{\text{CS}} &= \frac{23C_{2}(Z) - 576C_{2}(4Z) - 2187C_{2}(9Z) + 4096C_{2}(16Z) + 6S_{1}(Z) - 2S_{2}(Z) - 256S_{2}(4Z) + 4371S_{2}(9Z)}{7C_{2}(Z) - 1088C_{2}(4Z) + 9477C_{2}(9Z) - 2(6144C_{2}(16Z) + S_{1}(Z) - 2S_{2}(Z) + 128S_{2}(4Z))} \end{aligned} \tag{43} \\ \tilde{\alpha}_{2}^{\text{CS}} &= \frac{-5C_{2}(Z) - 960C_{2}(4Z) + 12393C_{2}(9Z) - 16384C_{2}(16Z) - 6S_{1}(Z) + 2S_{2}(Z) + 256S_{2}(4Z) - 4374S_{2}(9Z)}{7C_{2}(Z) - 1088C_{2}(4Z) + 9477C_{2}(9Z) - 2(6144C_{2}(16Z) + S_{1}(Z) - 2S_{2}(Z) + 128S_{2}(4Z))} \end{aligned} \tag{44} \\ \tilde{\beta}_{3}^{\text{CS}} &= \frac{2C_{2}(Z) - 384C_{2}(4Z) + 4374C_{2}(9Z) - 8192C_{2}(16Z) + 25S_{2}(Z) - 2560S_{2}(4Z) + 10935S_{2}(9Z)}{7C_{2}(Z) - 1088C_{2}(4Z) + 9477C_{2}(9Z) - 2(6144C_{2}(16Z) + S_{1}(Z) - 2S_{2}(Z) + 128S_{2}(4Z))} \end{aligned} \tag{45} \\ \tilde{\beta}_{4}^{\text{CS}} &= \frac{3(2C_{2}(Z) - 188C_{2}(4Z) + 9477C_{2}(9Z) - 8192C_{2}(16Z) + 25S_{2}(Z) - 2560S_{2}(4Z) + 10935S_{2}(9Z)}{7C_{2}(Z) - 1088C_{2}(4Z) + 9477C_{2}(9Z) - 2(6144C_{2}(16Z) + S_{1}(Z) - 2S_{2}(Z) + 128S_{2}(4Z))} \end{aligned} \tag{46}$$

We observe that in all five coefficient the power of Z in (13) is m = 3. As for the coefficients expressed in terms of $\eta_m(Z)$ functions, these are:

$$\tilde{\alpha}_{0}^{\eta} = \frac{-210\eta_{0}^{4}(Z/16) - 10\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) + \dots}{165\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) + \dots}$$
(47)

$$\tilde{\alpha}_{1}^{\eta} = \frac{630\eta_{0}^{4}(Z/16) + 315\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) - \dots}{165\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) + \dots}$$
(48)

$$\tilde{\alpha}_{2}^{\eta} = \frac{-90\eta_{0}^{4}(Z/16) - 45\eta_{0}^{2}(Z/64)(1 + eta_{0}(Z/16)) + \dots}{165\eta_{0}^{2}(Z/64)(1 + \eta_{0}(Z/16)) + \dots}$$
(49)

$$\tilde{\beta}_{3}^{\eta} = \frac{5(162\eta_{0}^{4}(Z/16) + 81\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) - \dots}{165\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) + \dots}$$
(50)

$$\tilde{\beta}_{4}^{\eta} = \frac{-3(90\eta_{0}^{4}(Z/16) + 45\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) - \dots}{165\eta_{0}^{2}(Z/64)(1+\eta_{0}(Z/16)) + \dots}$$
(51)

Similar to the previous case, the full expression of the coefficients can be obtained using the Mathematica modules in [30].

5 A check on the effectiveness of the approach

In this Section we show the graphs of the behavior of the coefficients and how our reformulation restores the convergence of the corresponding method.

On the left column of Fig. 1 we show the h dependence of the coefficients



Fig. 1. Left: Coefficients \tilde{c}_i^{ef} , \tilde{c}_i^{CS} , \tilde{c}_i^{η} of Example 1 for $\omega = 10$; **Right**: Error of \tilde{c}_i^{bf} and \tilde{c}_i^{CS} coefficients with respect to \tilde{c}_i^{η}

 $\tilde{c}_i^{\text{ef}}(\nu), \nu = \omega h$, for $\omega = 10$ and i = 0, 1, 2 of Example 1 compared with the reformulated $\tilde{c}_i^{\text{CS}}(Z), Z = -\nu^2 = -(\omega h)^2$, by means of C(Z) and S(Z) functions, and $\tilde{c}_i^{\eta}(Z)$ by means of $\eta_m(Z)$ functions. In particular, we observe that the coefficients expressed in terms of $\eta_m(Z)$ functions and the coefficients expressed in terms of C and S functions converge to the classical value, while the coefficients

 $\tilde{c}_0^{\text{eg}}, \tilde{c}_1^{\text{eg}}$ and \tilde{c}_2^{eg} blow up when h is decreased. From the numerical point of view the limit tendency (27) is not verified but (34) holds true.

On the right column of the same figure we give additional details. On it we present the deviations of the coefficients computed by the first two approaches with respect to those expressed in terms of the $\eta_m(Z)$ functions. It is seen that the two reformulations (28)–(30) and (31)–(33) differ by a factor of only 10^{-10} irrespective of h while the EF coefficients (24)–(26) exhibit an error which increases as $h \to 0$ to reach a value of about 10^2 for $h = 10^{-3}$.



Fig. 2. Left: Coefficients α_i^{ef} , α_i^{CS} , α_i^{η} of Example 2 for $\omega = 10$; **Right**: Error of α_i^{ef} , α_i^{CS} coefficients with respect to α_i^{η}

The same data are presented on Figs. 2–3 for the coefficients of Example 2. Again, the coefficients obtained in the frame of the original EF approach of

11



Fig. 3. Left: Coefficients β_i^{ef} , β_i^{CS} , β_i^{η} of Example 2 for $\omega = 10$; **Right**: Error of β_i^{ef} and β_i^{CS} coefficients with respect to β_i^{η}

[71] are oscillating and inaccurate when $h \rightarrow 0$, in contrast with those in the other two approaches. The results from the latter two approaches are actually in agreement within 10^{-15} .

Also instructive is that, in contrast with Example 1, the blow up of the original EF estimates occurs at values of h much smaller than before, and this is due to the power m in (13) which for the previous case was m = 4 while it is m = 3 by now. This allows concluding that the need of reformulations in the spirit of the approach presented in this paper is more and more stringent when m is increased.

An important issue is that of checking in what extent the accuracy in the evaluation of the coefficients affects the accuracy of the results when solving numerically a differential equation. To illustrate this we consider the following problem:

$$\begin{cases} y'' = -100y(t) + 99\sin(t) \\ y(0) = 1 \\ y'(0) = 11 \end{cases}$$
(52)

with $t \in [0, 20\pi]$, whose analytic solution is $y(t) = \cos(10t) + \sin(10t) + \sin(t)$. In Fig. 4, we compare the method (20)–(21) for three versions of the coefficients; in particular we denote:

- EF: the method with coefficients (23)-(24)-(25)-(26);

12 D. Conte et al.



Fig. 4. Absolute error in $t = 20\pi$ of method (20)–(21) on problem (52)

- EF converted CS: the method with coefficients (23)-(28)-(29)-(30) converted by means of C and S functions;
- EF converted $\eta_m(Z)$: the method with coefficients (23)–(31)–(32)–(33) converted by $\eta_m(Z)$ functions.

Fig. 4 shows that the reformulation of the coefficients in terms of either C and S or of η functions fully restores the convergence of the method.

6 Conclusions

We have shown that the reformulation of the expressions of the coefficients of EF-based numerical methods for differential equations in terms of the sets of functions C and S has two main advantages:

- 1. it allows reducing the original set of four expressions for each coefficient to a single one with universal use:
- 2. it removes completely the potential inaccuracy of the numerical solution when the step size h is small.

The procedure is then recommended as a reliable alternative to that based on η functions.

Further developments of this research will be oriented to the reformulation, through C and S functions, of existing methods for ordinary differential equations [2, 17, 20, 25, 26, 28, 37–39, 41, 42, 44, 49, 52, 54, 57, 79, 82], integral equations [5–8, 10, 11, 24, 29, 32, 34, 56, 73], stochastic problems [12, 13, 18, 19, 29, 47], fractional equations [12, 13, 21, 22, 36], partial differential equations [58–60, 68, 76].

References

- K. Burrage, A. Cardone, R. D'Ambrosio, B. Paternoster, Numerical solution of time fractional diffusion systems, Appl. Numer. Math. 116, 82–94 (2017).
- J. Butcher, R. D'Ambrosio, Partitioned general linear methods for separable Hamiltonian problems, Appl. Numer. Math. 117, 69–86 (2017).
- M. Calvo, J.M. Franco, J.I. Montijano, L. Rández, Explicit Runge-Kutta methods for initial value problems with oscillating solutions, J. Comput. Appl. Math. 76 (1-2), 195-212 (1996).
- M. Calvo, J.I. Montijano, L. Rández, M. Van Daele, Exponentially fitted fifth-order two step peer explicit methods, AIP Conf. Proc. 1648, 150015-1 – 150015-4 (2015).
- 5. G. Capobianco, D. Conte, An efficient and fast parallel method for Volterra integral equations of Abel type, J. Comput. Appl. Math., Vol 189/1-2 481-493 (2006).
- G. Capobianco, D. Conte, I. Del Prete, High performance numerical methods for Volterra equations with weakly singular kernels, J. Comput. Appl. Math., 228 (2009).
- G. Capobianco, D. Conte, B. Paternoster, Construction and implementation of twostep continuous methods for Volterra Integral Equations, Appl. Numer. Math. 119, 239-247 (2017)
- A. Cardone, D. Conte, Multistep collocation methods for Volterra Integro-Differential Equations, Appl. Math. Comput., 221, 770-785 (2013).
- A. Cardone, D. Conte, R. D'Ambrosio, B. Paternoster, Stability Issues for Selected Stochastic Evolutionary Problems: A Review, Axioms, doi: 10.3390/axioms7040091 (2018).
- A. Cardone, D. Conte, R. D'Ambrosio, B. Paternoster, Collocation Methods for Volterra Integral and Integro-Differential Equations: A Review, Axioms 7(3), 45 (2018).
- 11. A. Cardone, D. Conte, B. Paternoster, A family of Multistep Collocation Methods for Volterra Integro-Differential Equations, AIP Conf. Proc. 1168 (1), 2009.
- A. Cardone, D. Conte, B. Patenoster, Two-step collocation methods for fractional differential equations, Discr. Cont. Dyn. Sys. – B 23(7), 2709-2725 (2018).
- A. Cardone, R. D'Ambrosio, B. Paternoster, A spectral method for stochastic fractional differential equations, Appl. Numer. Math. 139, 115–119 (2019).
- 14. A. Cardone, R. D'Ambrosio, B. Paternoster, Exponentially fitted IMEX methods for advection-diffusion problems, J. Comput. Appl. Math. 316, 100–108 (2017).
- A. Cardone, R. D'Ambrosio, B. Paternoster, High order exponentially fitted methods for Volterra integral equations with periodic solution, Appl. Numer. Math. 114C,18–29 (2017).
- A. Cardone, L. Gr. Ixaru, B. Paternoster, Exponential fitting direct quadrature methods for Volterra integral equations, Numer. Algorithms 55, 467–480 (2010).
- V. Citro, R. D'Ambrosio, Nearly conservative multivalue methods with extended bounded parasitism, Appl. Numer Math., doi: 10.1016/j.apnum.2019.12.007 (2019).
- V. Citro, R. D'Ambrosio, S. Di Giovacchino, A-stability preserving perturbation of Runge-Kutta methods for stochastic differential equations, Appl. Math. Lett. 102, 106098 (2020).

- 14 D. Conte et al.
- V. Citro, R. D'Ambrosio, Long-term analysis of stochastic theta-methods for damped stochastic oscillators, Appl. Numer Math. 150, 18-26 (2020).
- R. D'Ambrosio, B. Paternoster, P-stable general Nystrom methods for y"=f(x,y), J. Comput. Appl. Math. 262, 271-280 (2014).
- D. Conte, G. Califano, Domain Decomposition Methods for a Class of Integro-Partial Differential Equations, AIP Conf. Proc. 1776, 090050 (2016).
- D. Conte, G. Califano, Optimal Schwarz Waveform Relaxation for fractional diffusion-wave equations, Appl. Numer. Math. 127, 125-141 (2018).
- Conte, D., D'Ambrosio, R., Giordano, G., Paternoster, B.: Regularized exponentially fitted methods for oscillatory problems. Journal of Physics: Conference Series, in press.
- D. Conte, R. D'Ambrosio, G. Izzo, Z. Jackiewicz, Natural Volterra Runge-Kutta methods, Numer. Algor. 65 (3), 421–445 (2014).
- D. Conte, R. D'Ambrosio, Z. Jackiewicz, B. Paternoster, A pratical approach for the derivation of algebraically stable two-step Runge-Kutta methods, Math. Model. Anal, 17 (1), 65-77 (2012).
- D. Conte, R. D'Ambrosio, Z. Jackiewicz, B. Paternoster, Numerical search for algebraically stable two-step almost collocation methods. J. Comput. Appl. Math. 239, 304-321 (2013).
- D. Conte, R. D'Ambrosio, M. Moccaldi, B. Paternoster, Adapted explicit two-step peer methods, J. Numer. Math. 27(2), 69–83 (2019).
- D. Conte, R. D'Ambrosio, B. Paternoster, GPU acceleration of waveform relaxation methods for large differential systems, Numer. Algor., 71(2), 293–310 (2016).
- D. Conte, R. D'Ambrosio, B. Paternoster, On the stability of θ-methods for stochastic Volterra integral equations, Discr. Cont. Dyn. Sys. - Series B 23(7), 2695– 2708 (2018).
- 30. Conte, D., Esposito, E., Ixaru, L.Gr., Paternoster, B.: Some new uses of the $\eta_m(Z)$ functions. Comput. Phys. Commun. 181, 128–137 (2010).
- D. Conte, L. Gr. Ixaru, B. Paternoster, G. Santomauro, Exponentially-fitted Gauss-Laguerre quadrature rule for integrals over an unbounded interval, J. Comput. Appl. Math. 255, 725–736 (2014).
- D. Conte, B. Paternoster, A Family of Multistep Collocation Methods for Volterra Integral Equations, AIP Conf. Proc. 936, 128-131 Springer (2007).
- D. Conte, B. Paternoster, Modified Gauss-Laguerre Exponential Fitting Based Formulae, J. Sc. Comp. 69 (1), 227—243 (2016).
- D. Conte, B. Paternoster, Parallel methods for weakly singular Volterra Integral Equations on GPUs, Appl. Numer. Math. 114,30-37 (2017).
- D. Conte, B. Paternoster, G. Santomauro, An exponentially fitted quadrature rule over unbounded intervals, AIP Conf. Proc. 1479, 1173–1176 Springer (2012).
- D. Conte, S. Shahmorad, Y. Talaei, New fractional Lanczos vector polynomials and their application to system of Abel–Volterra integral equations and fractional differential equations, J. Comput. Appl. Math. 366,112409 (2020).
- R. D'Ambrosio, G. De Martino, B. Paternoster, Numerical integration of Hamiltonian problems by G-symplectic methods, Adv. Comput. Math. 40(2), 553-575 (2014).
- R. D'Ambrosio, G. De Martino, B. Paternoster, Order conditions of general Nyström methods, Numer. Algor., 65(3) 579-595 (2014).
- R. D'Ambrosio, G. De Martino, B. Paternoster. General Nyström methods in Nordsieck form: error analysis, J. Comput. Appl. Math. 292, 694-702 (2016).

- R. D'Ambrosio, E. Esposito, B. Paternoster, Exponentially fitted two-step Runge-Kutta methods: Construction and parameter selection, Appl. Math. Comp. 218 (14), 7468–7480 (2012).
- R. D'Ambrosio, E. Hairer, Long-term stability of multi-value methods for ordinary differential equations, J. Sci. Comput. 60(3), 627-640 (2014).
- 42. R. D'Ambrosio, E. Hairer, C. Zbinden, G-symplecticity implies conjugatesymplecticity of the underlying one-step method, BIT Numer. Math. 53, 867-872 (2013).
- R. D'Ambrosio, L. Gr. Ixaru, B. Paternoster, Construction of the ef-based Runge-Kutta methods revisited, Comput. Phys. Commun. 182, 322-329 (2011).
- 44. R. D'Ambrosio, G. Izzo, Z. Jackiewicz, Search for highly stable two-step Runge-Kutta methods for ODEs, Appl. Numer. Math. 62(10), 1361-1379 (2012).
- 45. R. D'Ambrosio, M. Moccaldi, B. Paternoster, Adapted numerical methods for advection-reaction-diffusion problems generating periodic wavefronts, Comput. Math. Appl. 74(5), 1029–1042 (2017).
- 46. R. D'Ambrosio, M. Moccaldi, B. Paternoster, Parameter estimation in IMEXtrigonometrically fitted methods for the numerical solution of reaction-diffusion problems, Comp. Phys. Commun. 226, 55–66 (2018).
- 47. R. D'Ambrosio, M. Moccaldi, B. Paternoster, Numerical preservation of long-term dynamics by stochastic two-step methods, Discr. Cont. Dyn. Sys. - Series B 23(7), 2763–2773 (2018).
- R. D'Ambrosio, M. Moccaldi, B. Paternoster, F. Rossi, Adapted numerical modelling of the Belousov–Zhabotinsky reaction, J. Math. Chem., doi: 10.1007/s10910-018-0922-5 (2018).
- 49. R. D'Ambrosio, B. Paternoster, Exponentially fitted singly diagonally implicit Runge-Kutta methods, J. Comput. Appl. Math , 263, 277–287 (2014).
- 50. R. D'Ambrosio, B. Paternoster, Numerical solution of a diffusion problem by exponentially fitted finite difference methods. SpringerPlus 3:425 (2014).
- R. D'Ambrosio, B. Paternoster, A general framework for numerical methods solving second order differential problems. Math. Comput. Simul. 110(1), 113-124 (2015).
- 52. R. D'Ambrosio, B. Paternoster, Numerical solution of reaction-diffusion systems of λ - ω type by trigonometrically fitted methods, J. Comput. Appl. Math. 294, 436-445 (2016).
- 53. R. D'Ambrosio, B. Paternoster, Multivalue collocation methods free from order reduction, Journal of Computational and Applied Mathematics, 112515 (2019).
- 54. R. D'Ambrosio, B. Paternoster, G. Santomauro, Revised exponentially fitted Runge-Kutta-Nyström methods, Appl. Math. Lett., 30, 56–60 (2014).
- 55. De Bonis M.C, Occorsio D., On the simultaneous approximation of a Hilbert transform and its derivatives on the real semiaxis, Appl. Numer. Math. 114, 132–153 (2017).
- 56. Fang, J., Liu, C., Hsu, C.-W., Simos, T.E., Tsitouras, C.: Explicit hybrid six–step, sixth order, fully symmetric methods for solving y'' = f(x, y). Math. Meth. Appl. Sci., 42, 3305–3314 (2019).
- 57. Francomano, E., Paliaga, M. The smoothed particle hydrodynamics method via residual iteration, Computer Methods in Applied Mechanics and Engineering 352, 237–245 (2019).
- 58. M.R. Garvie, J.F. Blowey, A reaction-diffusion system of λ - ω type. Part II: Numerical analysis, Euro. J. Appl. Math. 16, 621–646 (2005).
- 59. J.M. Greenberg, Spiral waves for λ - ω systems, Adv. Appl. Math. 2, 450–455 (1981).
- Ixaru, L. Gr., Runge-Kutta method with equation dependent coefficients, Comput. Phys. Commun. 183, 63–69 (2012).

- 16 D. Conte et al.
- Ixaru, L. Gr.: Exponential and trigonometrical fittings: user-friendly expressions for the coefficients. Numerical Algorithms, 82, 1085–1096 (2019).
- 62. Ixaru, L.Gr., Vanden Berghe, G.: Exponential Fitting. Kluwer Academic Publishers, Dordrecht/Boston/London (2004).
- 63. L. Gr. Ixaru, B. Paternoster, A conditionally P-stable fourth-order exponentialfitting method for y'' = f(x, y) J. Comput. Appl. Math. 106 (1), (1999) 87–98.
- Ixaru, L. Gr., Paternoster, B., A Gauss quadrature rule for oscillatory integrands, Comput. Phys. Commun. 133, 177–188 (2001).
- Kim, J. K., Cools, R., Ixaru, L. Gr., Extended quadrature rules for oscillatory integrands, Appl. Numer. Math. 46, 59–73 (2003).
- Kim, J. K., Cools, R., Ixaru, L. Gr., Quadrature rules using first derivatives for oscillatory integrands, J. Comput. Appl. Math. 140, 479–497 (2002).
- N. Kopell, L.N. Howard, Plane wave solutions to reaction-diffusion equations, Stud. Appl. Math. 52, 291–328 (1973).
- 68. Liu, C., Hsu, C.W., Simos, T.E., Tsitouras, Ch.: Phase-fitted, six-step methods for solving x'' = f(t, x). Math. Meth. Appl. Sci., 42, 3942–3949 (2019).
- Montijano, J. I., Rández, L., Van Daele, M., Calvo, M., Functionally Fitted Explicit Two Step Peer Methods, J. Sci. Comput. 64(3), 938–958 (2014).
- Ndukum, P.L., Biala, T.A., Jator, S.N., Adeniyi, R.B.: On a family of trigonometrically fitted extended backward differentiation formulas for stiff and oscillatory initial value problems. Numer. Algor. 74, 267–287(2017).
- 71. Occorsio D, Russo M.G., Mean convergence of an extended Lagrange interpolation process on $[0, +\infty)$, Acta Mathematica Hungarica 142(2), 317–338 (2014).
- Occorsio D, Russo M.G., Nyström methods for Fredholm integral equations using equispaced points, Filomat 28(1), 49–63 (2014).
- Ozawa, K., A functional fitting Runge-Kutta method with variable coefficients, Jpn. J. Ind. Appl. Math. 18, 107-130 (2001).
- B. Paternoster, Present state-of-the-art in exponential fitting. A contribution dedicated to Liviu Ixaru on his 70-th anniversary, Comput. Phys. Commun. 183, 2499– 2512 (2012).
- M.J. Smith, J.D.M. Rademacher, J.A. Sherratt, Absolute stability of wavetrains can explain spatiotemporal dynamics in reaction-diffusion systems of lambda-omega type, SIAM J. Appl. Dyn. Systems 8, 1136–1159 (2009).
- Simos, T. E., A fourth algebraic order exponentially-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation, IMA Journ. of Numerical Analysis, 21, 919–931 (2001).
- 77. Simos, T. E., An exponentially-fitted Runge-Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions. Comput. Phys. Comm. 115, 1-8 (1998).
- Vanden Berghe, G., De Meyer, H., Van Daele, M., Van Hecke, T., Exponentially fitted explicit Runge-Kutta methods, Comput. Phys. Commun. 123, 7–15 (1999).
- Van Daele, M., Vanden Berghe, G., Vande Vyver, H. Exponentially fitted quadrature rules of Gauss type for oscillatory integrands. Appl. Numer. Math. 53, 509–526 (2005).
- Van Daele, M., Van Hecke, T., Vanden Berghe, G., De Meyer, H., Deferred correction with mono-implicit Runge-Kutta methods for first-order IVPs, Numerical methods for differential equations, J. Comput. Appl. Math. 111 (1-2), 37-47 (1999).
- Weiner, R., Biermann, K., Schmitt, B. A., Podhaisky, H., Explicit two-step peer methods, Computers and Mathematics with Applications 55, 609-619 (2008).
- 82. https://en.wikipedia.org/wiki/Stumpff_function