Exponentially fitted singly diagonally implicit Runge-Kutta methods

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Abstract

It is the purpose of this paper to derive diagonally implicit exponentially fitted (EF) Runge-Kutta methods for the numerical solution of initial value problems based on first order ordinary differential equations, whose solutions are supposed to exhibit an exponential behaviour. In addition to the standard approach for the derivation of EF methods, we provide a revised constructive technique that takes into account the contribution to the error inherited from the computation of the internal stages. The derived methods are then compared to those obtained by neglecting the contribution of the error associated to the internal stages, as classically done in the standard derivation of multistage EF-based methods. Standard and revised EF methods are then compared in terms of linear stability and numerical performances.

Key words: Ordinary differential equations, diagonally implicit methods, exponential fitting.

1. Introduction

It is the purpose of this paper to introduce special purpose semi-implicit Runge-Kutta (RK) methods for the numerical solution of ordinary differential equations (ODEs)

$$\begin{cases} y'(x) = f(x, y(x)), \quad x \in [x_0, X], \\ y(x_0) = y_0 \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

where $f : [x_0, X] \times \mathbb{R}^d \to \mathbb{R}^d$ is a sufficiently smooth function ensuring that the corresponding problem is well posed. The class of methods we aim to consider is the family of singly diagonally implicit Runge-Kutta (SDIRK) methods

$$\begin{cases} y_{n+1} = y_n + h \sum_{i=1}^{m} b_i f(x_n + c_i h, Y_i^{[n]}), \\ Y_i^{[n]} = y_n + h \sum_{j=1}^{i} a_{ij} f(x_n + c_j h, Y_j^{[n]}), \quad i = 1, 2, \ldots, m, \end{cases} \tag{1.2}$$

conventionally represented in terms of their Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cccc} c_1 & a_{11} & & & \\ c_2 & a_{21} & a_{22} & & \\ \vdots & \vdots & \vdots & \ddots & \\ c_m & a_{m1} & a_{m2} & \cdots & a_{mm} \\ \hline & b_1 & b_2 & \cdots & b_m \end{array},$$

where all the diagonal elements a_{ii}, $i = 1, 2, \ldots, m$, are all equal to a common value $\lambda \in \mathbb{R}$.

It is known from the literature that the lower triangular structure of the matrix A allows to solve the md-dimensional nonlinear system in (1.2) in m forward steps, each consisting in the solution of a d-dimensional nonlinear system. Moreover, if all the elements on the diagonal are equal, in solving the nonlinear systems by means of Newton-type iterations, the repeated use of the stored LU factorization of the Jacobian is made possible. If the matrix A is diagonal, the nonlinear system can also be solved in a parallel computational environment (see, for instance, [2, 23]).

Within the class of RK methods (1.2), we aim to introduce a family of formulae depending on non-constant coefficients for the numerical solution of (1.1) whose solution is supposed to exhibit a prominent exponential behaviour. Classical numerical methods for ODEs may not be well-suited to follow a prominent exponential or oscillatory behaviour of the solutions, because a very small stepsize would be required, with corresponding deterioration of the numerical performances, especially in terms of efficiency. One of the possible ways to proceed in order to derive numerical methods particularly tuned to the behaviour of the solution can be realized by imposing that a numerical method exactly integrates (within the round-off error) problems of type (1.1) whose solution can be expressed as linear combination of functions other than polynomials: this is the spirit of the exponential fitting (EF) technique (compare [26, 31] and references therein), where the *adapted* numerical method is developed in order to exactly solve problems whose solution belongs to the linear space spanned by

$$\{1, x, \ldots, x^K, \exp(\pm\mu x), x\exp(\pm\mu x), \ldots, x^P \exp(\pm\mu x)\},$$

with K and P integer numbers. When μ is purely imaginary, the oscillatory case is also recovered.

EF-based adaptations of both explicit and implicit RK formulae have been introduced in [34, 37] and later on investigated, for instance, in [3, 15, 28, 29, 35, 36, 38, 39] and references therein, also for second order ODEs [20, 21, 29, 31] and the Schrödinger equation [1]. Such methods reveal to be a valid alternative to classical methods shaped on algebraic polynomial basis (compare, for instance [2, 7, 8, 12, 16, 17, 18, 19], and references therein), when the problem exhibits a non-polynomial behaviour. For an updated state-of-the art on exponential fitting, compare [31]. Further adaptations of other families of multistage methods are object of [4, 11, 13, 14, 15, 32, 33]

Here we focus our attention on the derivation of two different EF versions of (1.2): the first one, in accordance to the standard EF technique [26], is derived by assuming that the values of the approximations inherited from the computation of the internal

stages are exact and, thus, they do not provide any further contribution to the discretization error of the overall scheme; the second version, which follows the spirit of [10, 25], instead takes into account the error provided by the internal stages computation, which cumulates to the truncation error of the overall scheme. Later on, we refer to the former version as *standard* EF-technique, while the latter is denoted as *revised* EF-technique.

EF-based RK methods (1.2) depend on the value of a parameter to be suitably determined. The estimation of the unknown parameter is, in general, a nontrivial problem. In fact, up to now, a rigorous theory for the exact computation of the parameter has not yet been developed, but several attempts have been done in the literature (see, for instance, [24, 26, 27] and references therein contained) in order to provide an accurate estimation. In this paper, following the spirit of [37], we approximate the value of the unknown parameter by minimizing the leading term of the local discretization error.

The paper is organized as follows: Section 2 presents theoretical arguments for the EF adaptation of a diagonally implicit RK methods, according to the standard EF technique; Section 3 introduces a revisitation of this technique, taking into account the multistage nature of the solver in a deeper way; Section 4 provides examples of both standard and revised singly diagonally implicit RK methods. The numerical evidence is reported in Section 5, while some conclusions are reported in Section 6.

2. Standard EF-based SDIRK methods

The building blocks employed in the standard constructive technique for the derivation of EF-based multistage methods (compare [6, 26]) are based on the following $m+1$ functional operators

$$\mathcal{L}[h, \mathbf{b}]y(x) = y(x+h) - y(x) - h\sum_{i=1}^{m} b_i y'(x+c_i h), \tag{2.3}$$

$$\mathcal{L}_i[h, \mathbf{a}]y(x) = y(x+c_i h) - y(x) - h\sum_{j=1}^{i} a_{ij} y'(x+c_j h), \quad i = 1, \ldots, m, \tag{2.4}$$

respectively associated to the first and second equation in (1.2). In particular, the $\mathcal{L}$ operator is associated to the so called external stage, i.e. the approximation y_{n+1} of the solution in the point x_{n+1}, while each operator $\mathcal{L}_i$ is connected to the internal approximation Y_i of $y(x_n + c_i h)$, also denoted as internal stage.

We aim to derive methods able to exactly solve ODE based problems (1.1), whose solutions belong to the linear space spanned by

$$\mathcal{F} = \{1, \exp(\mu x), x\exp(\mu x), \ldots, x^P \exp(\mu x)\},$$

where P is a suitable integer number. We observe that, in this basis, monomials are absent (i.e. $K = 0$): this choice is due to the fact that we aim to derive methods which are more exponentially fitted, thus more suited to integrate differential problems with non-polynomial solutions.

We first analyze the set of conditions that the weights b_i of the RK method (1.2) have to satisfy in order to annihilate the operator (2.3), for any function belonging to

$\mathcal{F}$. We introduce the matrices C, D whose entries are given by

$$c_{ij} = jc_i^{j-1}, \quad i = 1, 2, \ldots, m, \ j = 1, 2, \ldots, P,$$

$$d_{ij} = c_i^j, \quad i = 1, 2, \ldots, m, \ j = 1, 2, \ldots, P,$$

and the matrix $E = \mathrm{diag}(e^{cz})$, where the vector e^{cz} denotes the componentwise exponentiation of the abscissa vector c. Then, the following result holds.

Theorem 2.1. *Suppose that the weights vector b of the RK method* (1.2) *satisfy the algebraic constraints*

$$\begin{cases} b^T e^{cz} = \dfrac{e^z - 1}{z}, \\ b^T E(C + Dz) = e^z \mathbf{1}, \end{cases} \tag{2.5}$$

where $z = \mu h$ and $\mathbf{1}$ denotes the unit vector in $\mathbb{R}^P$. Then, the linear operator (2.3) *is identically equal to zero for any function belonging to $\mathcal{F}$.*

Proof: We annihilate the linear operator (2.3) in correspondence of the elements of the functional basis $\mathcal{F}$. The operator is identically zero when $y(x) = 1$ while, in correspondence of $y(x) = \exp(\mu x)$, it annihilates if

$$\exp(z) - 1 - z \sum_{i=1}^{m} b_i \exp(c_i z) = 0.$$

If $y(x) = x^k \exp(\mu x)$, for $k = 1, 2, \ldots, P$, then the operator (2.3) is identically equal to zero provided that the weights b_i satisfy the algebraic constraints

$$\exp(z) - \sum_{i=1}^{m} b_i c_i^{k-1}(k + c_i z) \exp(c_i z) = 0, \quad k = 1, 2, \ldots, P.$$

By collecting such conditions in matrix form, the result is obtained. □

We observe that if $P = m - 1$, the linear system resulting from (2.5) has a unique solution: this can be proved by observing that the determinant of its coefficient matrix is related to that of a Vandermonde matrix (compare, for instance, Theorem 2.1 in [15]). Hence, the following corollary holds.

Corollary 2.1. *If $P = m - 1$, then the weights of the EF-based RK method corresponding to the fitting space $\mathcal{F}$ are the solution of linear system* (2.5)*.*

We observe that, when z tends to 0, conditions (2.5) recover the classical subset of order conditions

$$\sum_{i=1}^{m} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, 2, \ldots, m,$$

for RK methods, associated to the bushy trees $[\tau]_k$, reported for instance in [2, 22].

By analogous arguments, we obtain the following result for the elements of the coefficient matrix A.

Theorem 2.2. *Suppose that the matrix A of the RK method* (1.2) *satisfy the algebraic constraint*

$$\begin{cases} Ae^{cz} = \dfrac{e^z - 1}{z}\mathbf{1}, \\ AE(C + zD) = D. \end{cases} \tag{2.6}$$

Then, the linear operators (2.4) *annihilate on the functional set* $\mathcal{F}$.

Proof: Following the lines drawn in the proof of Theorem 2.1, we annihilate the linear operators (2.4) on the fitting space $\mathcal{F}$. They are all identically equal to zero when $y(x) = 1$ while, in correspondence of $y(x) = \exp(\mu x)$, they annihilates if

$$\exp(c_i z) - 1 - z\sum_{j=1}^{i} a_{ij}\exp(c_i z) = 0, \qquad i = 1, 2, \ldots, m.$$

If $y(x) = x^k \exp(\mu x)$, for $k = 1, 2, \ldots, P$, then the operators (2.4) are identically zero provided that the algebraic conditions

$$c_i^k - \sum_{j=1}^{i} a_{ij} c_j^{k-1}(k + c_j z)\exp(c_j z) = 0, \quad i = 1, 2, \ldots, m, \quad k = 1, 2, \ldots, P,$$

are satisfied. By collecting such conditions in matrix form, the result is obtained. □

We observe that if $P = m - 1$, the linear system (2.6) has a unique solution, by similar arguments to those the b vector. Thus, the following corollary holds.

Corollary 2.2. *If* $P = m - 1$, *then the weights of the EF-based RK method corresponding to the fitting space* $\mathcal{F}$ *are the solution of linear system* (2.6).

We observe that, when z tends to 0, conditions (2.6) recover the classical simplifying assumptions

$$\sum_{j=1}^{i} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \qquad i = 1, 2, \ldots, m, \quad k = 1, 2, \ldots, q,$$

for RK methods [2, 22], being q the stage order of the method.

3. Revised EF-based SDIRK methods

In standard derivations of EF Runge-Kutta methods, the elements b_i of the weights vector are computed with the underlying assumption that

$$Y_i = y(x_n + c_i h),$$

i.e. the error in the computation of the internal stages is completely neglected. Our aim is now that of deriving EF-based methods where the influence of the error inherited by

the computation of the internal stages is taken into account. This investigations follows the spirit of [10, 25].

We denote by

$$\varepsilon_i = Y_i - y(x_n + c_i h), \qquad i = 1, 2, \ldots, m, \tag{3.7}$$

the error associated to the internal approximations. The stage errors (3.7) are generally non-zero and, thus, we want to consider their contribution to the error associated to the overall integration process. We consider the local error associated to the external stage y_{n+1} in (1.2)

$$\mathcal{L}^R[h, \mathbf{b}]y(x)\Big|_{x=x_n} = y(x_n + h) - y(x_n) - h \sum_{i=1}^{m} b_i^R f(x_n + c_i h, Y_i), \tag{3.8}$$

where the superscript R denotes that we are considering *revised* EF methods. Taking into account that

$$y'(x_n + c_i h) = f(x_n + c_i h, Y_i - \varepsilon_i) = f(x_n + c_i h, Y_i) - \varepsilon_i f_y(x_n + c_i h, Y_i) + O(\varepsilon_i^2) \tag{3.9}$$

we obtain

$$\mathcal{L}^R[h, \mathbf{b}]y(x)\Big|_{x=x_n} = y(x_n+h)-y(x_n)-h \sum_{i=1}^{m} b_i^R \left(y'(x_n + c_i h) + f_y(x_n + c_i h, Y_i)\varepsilon_i\right). \tag{3.10}$$

Hereinafter $f_y^{(i)}$ is the short-hand notation for $f_y(x_n + c_i h,\ Y_i)$.

We observe that, for $\varepsilon = 0$, we recover the expression of the standard error operator (2.3). The practical derivation of revised RK methods and the comparison of such methods with respect to the standard ones in terms of stability and numerical results is object of the following sections.

4. Derivation of two-stage SDIRK methods

We now derive examples of singly diagonally implicit SDIRK methods (1.2) by both applying the standard and the revised techniques presented in the previous section. The methods we are going to present are all depending on the values of two internal stages.

We first focus our attention on the family of standard EF-based SDIRK methods (1.2) with $m = 2$, by applying the results derived in Section 2. In this case, the linear operators (2.3) and (2.4) associated to (1.2) are

$$\begin{aligned}
\mathcal{L}[h, \mathbf{b}]z(x) &= z(x_n + h) - z(x) - h\left(b_1 z'(x + c_1 h) + b_2 z'(x + c_2 h)\right), \\
\mathcal{L}_1[h, \mathbf{a}]y(x) &= y(x_n + c_1 h) - y(x) - h\lambda y'(x + c_1 h), \\
\mathcal{L}_2[h, \mathbf{a}]y(x) &= y(x_n + c_2 h) - y(x) - h\left(a_{21} y'(x + c_1 h) + \lambda y'(x + c_2 h)\right).
\end{aligned}$$

Due to the results carried out in Section 2, the fitting spaces we have to consider are

$$\hat{\mathcal{F}} = \{1, e^{\mu x}, x e^{\mu x}\}, \qquad \mathcal{F} = \{1, e^{\mu x}\}, \tag{4.11}$$

which are respectively associated to the external and internal stages computation: i.e. the external value is exact on the linear space generated by $\hat{\mathcal{F}}$, while the internal stages approximations are exact on the linear space spanned by $\mathcal{F}$. Thus, we next derive the coefficients λ, a_{21}, b_1 and b_2 by imposing that

$$\mathcal{L}_i[h, \mathbf{a}]z(x) = 0, \quad i = 1, 2, \quad \text{for any } z(x) \in \mathcal{F},$$

and

$$\mathcal{L}[h, \mathbf{b}]z(x) = 0, \quad \text{for any } z(x) \in \hat{\mathcal{F}},$$

or, equivalently, by means of Theorems 2.1 and 2.2. We obtain

$$\lambda = \frac{1 - e^{-c_1 z}}{z}, \quad a_{21} = \frac{e^{c_2 z} - e^{c_1 z}}{z e^{2c_1 z}},$$

$$b_1 = \frac{1 + c_2 z + e^z(-1 + z - c_2 z)}{(c_1 - c_2) z^2 e^{c_1 z}}, \quad b_2 = -\frac{1 + c_1 z - e^z(1 - z + c_1 z)}{(c_1 - c_2) z^2 e^{c_2 z}},$$

with $z = \mu h$. We observe that the methods belonging to the derived family have order 2 since, for z tending to 0, they satisfy the set of conditions

$$\sum_{i=1}^{2} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, 2,$$

guaranteeing order 2 for RK methods depending on two stages [2, 22].

We next derive the coefficients of the revised EF-based SDIRK methods, by assuming that the fitting spaces $\mathcal{F}$ and $\widehat{\mathcal{F}}$ are the same as in the standard case. The internal stage approximations result to be exact on the intersection set

$$\mathcal{F} \cap \widehat{\mathcal{F}} = \{1, \ \exp(\mu x)\}.$$

Since these two functions are solutions of the differential equation

$$y'' - \mu y' = 0,$$

the leading term of the error in the computation of each internal stage is

$$\varepsilon_i = Y_i - y(x_n + c_i h) = h^2 F_i (y''(x_n) - \mu y'(x_n)) + O(h^3), \quad i = 1, 2, \tag{4.12}$$

where F_i is the i-th stage error constant. The stage errors (4.12) are generally non-zero and, thus, we want to consider their contribution to the error associated to the overall integration process. The knowledge of these errors needs the calculation of the values of the stage error constants F_i in (4.12): this is done by following the procedure used in [10, 25], i.e. by solving the linear system

$$\mathcal{L}_i[h, \mathbf{a}]x = \varepsilon_i\Big|_{y(x)=x}, \quad i = 1, 2,$$

with respect to F_1 and F_2, where ε_i is defined in (4.12). The obtained values are

$$F_i = \frac{\sum_{j=1}^{2} a_{ij} - c_i}{z}. \tag{4.13}$$

We next consider the revised linear operator (3.10)

$$\mathcal{L}^R[h,\mathbf{b}]y(x)\Big|_{x=x_n} = y(x_n+h) - y(x_n) - h\sum_{i=1}^{2} b_i^R\left(y'(x_n+c_ih) - f_y(x_n+c_ih,Y_i)\varepsilon_i\right),$$

and evaluate it in correspondence to the elements of $\mathcal{F}$ in (4.11): in particular, we observe that $\mathcal{L}^R[h,\mathbf{b}]1$ is automatically equal to zero, while the requested values of $b_1^R(z)$ and $b_2^R(z)$ are those satisfying

$$\mathcal{L}^R[h,\mathbf{b}]e^{\mu x}\Big|_{x=0} = \mathcal{L}^R[h,\mathbf{b}]xe^{\mu x}\Big|_{x=0} = 0,$$

i.e.

$$b_1^R(z) = \frac{\alpha(z)z^3b_1 + e^{-c_1z}\left(-1+e^z\right)f_y^{(2)}h\left(-2e^{c_1z}+e^{c_2z}+e^{2c_1z}\left(1-c_2z\right)\right)}{\alpha(z)z^3+\beta(z)hz}, \tag{4.14}$$

$$b_2^R(z) = \frac{\alpha(z)z^3b_2 + \left(-1+e^z\right)f_y^{(1)}h\left(1+e^{c_1z}\left(-1+c_1z\right)\right)}{\alpha(z)z^3+\beta(z)hz}, \tag{4.15}$$

where

$$\alpha(z) = (c_1-c_2)\,e^{(2c_1+c_2)z},$$

$$\beta(z) = \left(-2e^{c_1z}f_y^{(2)} + e^{c_2z}\left(f_y^{(1)}+f_y^{(2)}\right) + e^{(c_1+c_2)z}f_y^{(1)}\left(-1+c_1z\right) + e^{2c_1z}f_y^{(2)}\left(1-c_2z\right)\right).$$

Thus, the parameters of the methods are now completely determined. We observe that the coefficients of the revised methods depend on evaluations of the partial derivative of f with respect to y that, in the following sections, are assumed to be computed by exact differentiation of the vectorial field in (1.1).

4.1. The case of differential systems

We have introduced so far a technique for the derivation of revised EF methods suited to integrate scalar problems. We now turn our attention to the case of system of equations, by deriving the version of method (4.14)-(4.15) applicable to integrate differential systems.

Taking into account that, in the case of systems, (3.9) has to be formulated as follows

$$y'(x_n+c_ih) = f(x_n+c_ih,Y_i+\varepsilon_i) = f(x_n+c_ih,Y_i) + \varepsilon_i J(x_n+c_ih,Y_i) + O(\varepsilon_i^2),$$

where J is the Jacobian of the vector field, the revised operator now assumes the form

$$\mathcal{L}^R[h,\mathbf{b}]y(x)\Big|_{x=x_n} = y(x_n+h) - y(x_n) - h\sum_{i=1}^{m} b_i^R\left(y'(x_n+c_ih) - J(x_n+c_ih,Y_i)\varepsilon_i\right). \tag{4.16}$$

Then, we assume as fitting space the analog of (4.11), i.e.

$$\mathcal{F} = \{\mathbf{1},\ e^{\mu x}\mathbf{1},\ xe^{\mu x}\mathbf{1}\},$$

being **1** the vector of ones having the dimension of the differential problem, and evaluate (4.16) on them. This gives, in case of two stage methods, the following revised coefficients

$$b_1^R(z) = \Gamma(z)(\alpha(z)z^3 b_1 I + e^{-c_1 z}(-1+e^z)\, h\left(-2e^{c_1 z} + e^{c_2 z} + e^{2c_1 z}(1-c_2 z)\right) J^{(2)}, \quad (4.17)$$

$$b_2^R(z) = \Gamma(z)(\alpha(z)z^3 b_2 I + (-1+e^z)\, h\,(1 + e^{c_1 z}(-1+c_1 z))\, J^{(1)}, \quad (4.18)$$

where $\Gamma(z) = \left(\alpha(z)z^3 I + \Lambda(z)hz\right)^{-1}$, being

$$\Lambda(z) = \left(-2e^{c_1 z} J^{(2)} + e^{c_2 z}\left(J^{(1)} + J^{(2)}\right) + e^{(c_1+c_2)z} J^{(1)}(-1+c_1 z) + e^{2c_1 z} J^{(2)}(1-c_2 z)\right).$$

In the above expression, we have used the shorthand notation $J^{(i)}$ to denote $J(x_n + c_i h, Y_i)$, $i = 1, 2$.

5. Linear stability analysis

We next consider the linear stability analysis of the derived methods with respect to the classical test problem $y' = \omega y$, with $\mathrm{Re}(\omega) < 0$, as done in [5]. The application of a RK method to such problem leads to the recurrence relation $y_{n+1} = R(\nu, z)y_n$, where

$$R(\nu, z) = 1 + \nu \mathbf{b}^T(z)(I - \nu \mathbf{A}(z))^{-1}\mathbf{e},$$

is the stability function of the method, being $\mathbf{e} \in \mathbb{R}^s$ the unit vector. In correspondence to this notion, we recall the following definition of stability region [10].

Definition 5.1. *The region of the three-dimensional* $(\mathrm{Re}(\nu), \mathrm{Im}(\nu), z)$ *space on which the inequality*

$$|R(\nu, z)| < 1 \quad (5.19)$$

is satisfied is called a region of stability Ω *for the EF-based method* (1.2)*.*

Figures 1 and 2 present a selection of sections through the stability region by planes where z is constant, for fixed values of the nodes $c_1 = 0$ and $c_2 = 1$: we can advise from the picture that the regions corresponding to revised EF methods are larger than those corresponding to standard EF methods. Such a behaviour is more and more visible when the exponential behaviour of the solution becomes more prominent.

6. Numerical experiments

We finally provide a numerical evidence to assert the effectiveness of our approach, by considering the numerical solution of the nonlinear equation

$$\begin{cases} y'(x) = \dfrac{\lambda y^2(x) + 2x^3 e^{2\lambda x}}{y(x)}, \\ y(1) = e^{\lambda}, \end{cases} \quad (6.20)$$

with $x \in [1, 5]$, whose exact solution is $y(x) = x^2 e^{\lambda x}$ does not belong to the space $\mathcal{F} \cap \hat{\mathcal{F}}$, thus the derived methods are unable to solve these problems exactly.

We compare the following solvers:

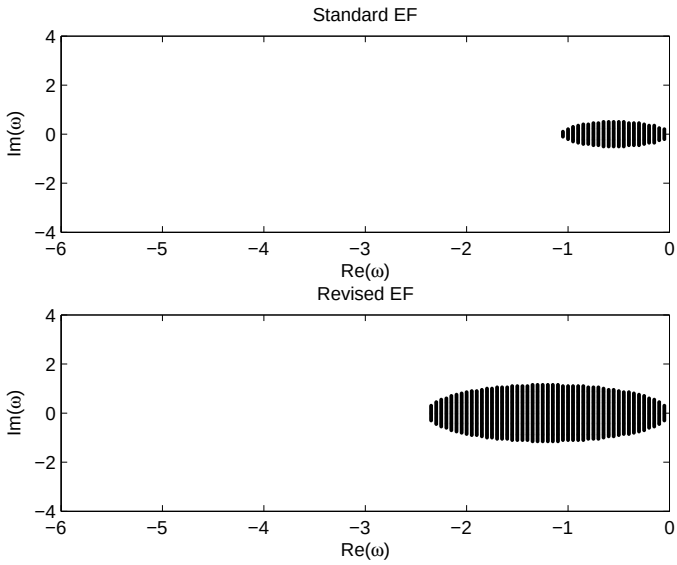

Figure 1: Section through the stability regions by plane $z = -2$ for (1.2), with $c_1 = 0$, $c_2 = 1$

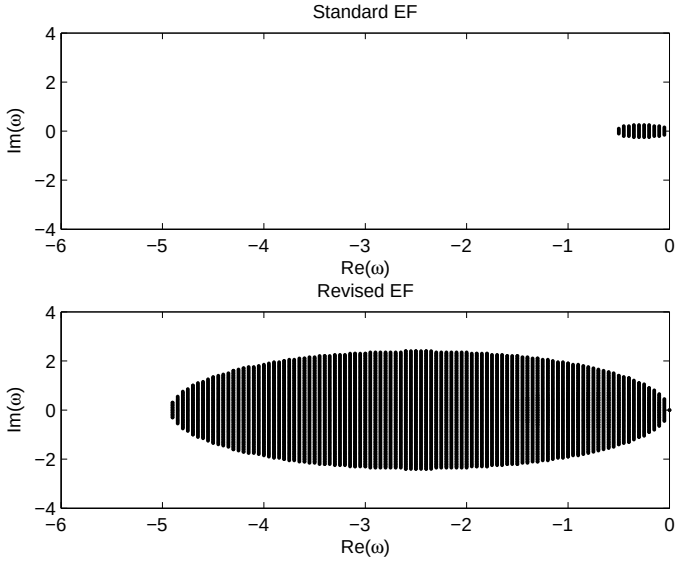

Figure 2: Section through the stability regions by plane $z = -4$ for (1.2), with $c_1 = 0$, $c_2 = 1$

- the classical second order SDIRK method (compare [2])

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cc} c_1 & c_1 & \\ c_2 & c_2 - c_1 & c_1 \\ \hline & \dfrac{1-2c_2}{2c_1-2c_2} & -\dfrac{1-2c_1}{2c_1-2c_2} \end{array}$$

- its standard EF adaptation

$$\begin{array}{c|c} c & A(z) \\ \hline & b^T(z) \end{array} = \begin{array}{c|cc} c_1 & \dfrac{1-e^{-c_1 z}}{z} & \\ c_2 & \dfrac{e^{c_2 z}-e^{c_1 z}}{z e^{2c_1 z}} & \dfrac{1-e^{-c_1 z}}{z} \\ \hline & \dfrac{1+c_2 z+e^z(-1+z-c_2 z)}{(c_1-c_2)z^2 e^{c_1 z}} & \dfrac{-1-c_1 z+e^z(1+(-1+c_1)z)}{(c_1-c_2)z^2 e^{c_2 z}} \end{array}$$

- its revised EF adaptation

$$\begin{array}{c|c} c & A(z) \\ \hline & b^T(z,\, f_y) \end{array} = \begin{array}{c|cc} c_1 & \dfrac{1-e^{-c_1 z}}{z} & \\ c_2 & \dfrac{e^{c_2 z}-e^{c_1 z}}{z e^{2c_1 z}} & \dfrac{1-e^{-c_1 z}}{z} \\ \hline & b_1^R & b_2^R \end{array}$$

  with b_1^R, b_2^R of the forms (4.14) and (4.15), respectively, in case of scalar problems. In the case of systems, b_1^R and b_2^R have the forms (4.17) and (4.18).

In both the standard and the revised EF methods, we compute at each step point the value $z = \mu_n h$, where μ_n is the fitted parameter approximated by the formula (compare [37])

$$\mu_n = \sqrt{-\frac{y''(x_n)}{y(x_n)}},$$

which provides a minimizer for the leading error term.

The computations have been done on a node with CPU Intel Xeon 6 core X5690 3,46GHz, belonging to the E4 multi-GPU cluster of Mathematics Department of Salerno University. The results, reported in Table 1, suggest that both the EF adaptations are able to approach the problem in a more accurate way than the classical SDIRK method of the same order. Moreover, by integrating both methods with the same constant step-size h, the revised EF method is generally more accurate than the standard one: the more the exponential behaviour is prominent, the more the superiority of the revised adaptation is evident. Table 2 reports the numerical evidence originated by applying the order 2 EF-based RK method

λ	h	err^C	cd^C	err^S	cd^S	err^R	cd^R
-2	2	6.58e-1	0.18	2.80e-2	1.55	1.83e-3	2.74
	1	1.14e-1	0.94	8.36e-3	2.08	3.08e-4	3.51
	1/2	2.14e-3	2.67	2.03e-3	2.69	1.84e-5	4.73
	1/4	1.33e-4	3.88	6.33e-5	4.20	3.82e-6	5.42
-4	2	unstable		1.14e-3	2.94	2.64e-6	5.58
	1	unstable		4.47e-7	6.32	9.77e-8	7.01
	1/2	unstable		3.05e-7	6.51	1.23e-7	6.91
	1/4	4.16e-6	5.38	3.77e-8	7.42	2.74e-8	7.56
-8	2	unstable		1.82e-2	1.74	8.81e-12	11.05
	1	unstable		1.30e-6	5.89	4.93e-10	9.31
	1/2	unstable		1.77e-7	6.75	5.45e-11	10.26
	1/4	2.41e-4	3.62	3.23e-7	6.49	3.95e-15	14.40

Table 1: Numerical results originated from the application of classical, EF-standard and EF-revised SDIRK method with two-stages and order 2, to problem (6.20) for different values of the parameter λ and of the step-size h. err^C and cd^C denote the global error and the number of gained correct digits for the classical SDIRK method, respectively, while err^S, cd^S, err^R and cd^R are analogous quantities associated to the standard and the revised EF-based methods, respectively

$$\begin{array}{c|c|cc} 0 & 1 & & \\ 1 & \cos(z) & \dfrac{\sin(z)}{z} & \\ \hline & & \dfrac{\sin(z)}{z(\cos(z)+1)} & \dfrac{\sin(z)}{z(\cos(z)+1)} \end{array} \tag{6.21}$$

derived in [37]. The spirit of this test is that of comparing two methods having the same order of convergence, both exponentially fitted on fitting spaces which do not contain the exact solution of problem (6.20). The numerical evidence reveals a better accuracy of our EF-based adaptation of the RK methods. Also in this case we observe that the more the exponential behaviour is prominent, the more the superiority of our revised EF method is visible, also when compared to other EF-based multistage formulae.

We next consider the following linear system

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \end{bmatrix} = \begin{bmatrix} \lambda & 2 \\ \frac{1}{x^2} & \lambda \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix}, \tag{6.22}$$

with $x \in [1, 5]$, whose exact solution is

$$y(x) = [x^2 e^{\lambda x}, x e^{\lambda x}]^T.$$

λ	h	err	cd
-2	1/2	2.24e-2	1.65
	1/4	4.69e-4	3.33
-4	1/2	4.92e-1	0.31
	1/4	1.49e-5	4.83
-8	1	6.01e-4	3.22
	1/4	2.41e-1	0.62

Table 2: Numerical results originated from the application of the EF method (6.21) of order 2, for different values of the parameter λ and of the stepsize h. err and cd denote the global error and the number of gained correct digits, respectively

The results are reported in Table 3. We observe that, for increasing values of the parameters, the results originated by the standard methods are very inaccurate, and the method itself does not exhibit its theoretical order of convergence. This is not the case of the revised method, which preserve its order convergence even for high values of the parameter.

We conclude this section presenting the numerical results obtained for the nonlinear system

$$\begin{cases} y_1'(x) = 3\,(y_2(x) - x) + \dfrac{\lambda y_1^2(x)}{x^3 e^{\lambda x}}, \\ y_2'(x) = \dfrac{y_2(x)\left(x^2 + 2y_1(x) + \lambda x^2 y_2(x) - \lambda x^3\right)}{x^3(1 + xe^{\lambda x})}, \\ y_1(1) = e^{\lambda},\ y_2(1) = 1 + e^{\lambda}, \end{cases} \tag{6.23}$$

for $x \in [1, 3]$, whose exact solution is

$$y(x) = [x^3 e^{\lambda x},\ x(1 + xe^{\lambda x})]^T.$$

The results obtained for several values of λ are collected in Table 4. Also in this case we realize that, the more the exponential behaviour is prominent, the more the superiority of the revised method is visible.

7. Conclusions

We have introduced in this paper singly diagonally implicit Runge-Kutta methods adapted for the solution of differential problems with a prominent exponential behaviour. Such adaptation is provided by means of the exponential fitting theory, which is properly extended to the case object of study. At the best of our knowledge, this is the first attempt of introducing EF-based Runge-Kutta methods depending on structured coefficient matrices. Due to the multistage nature of the methods, we have introduced not only the standard constructive approach, but also a revised one which takes into account the contribution of the error inherited by the computation of the internal stages. The superiority of the revised methods with respect to the standard

λ	h	err^S	cd^S	err^R	cd^R
-4	1/32	2.83e-1	0.55	7.81e-3	2.11
	1/64	1.64e-1	0.78	2.03e-3	2.69
	1/128	9.25e-2	1.03	5.14e-4	3.29
	1/256	5.16e-2	1.29	1.29e-4	3.89
-8	1/32	9.75e-1	0.01	4.77e-2	1.32
	1/64	8.14e-1	0.09	1.15e-2	1.94
	1/128	5.59e-1	0.25	2.83e-3	2.55
	1/256	3.35e-1	0.47	7.04e-4	3.15
-16	1/32	9.99e-1	5.75e-12	5.72e-1	0.24
	1/64	9.99e-1	3.90e-5	1.80e-1	0.74
	1/128	9.84e-1	7.02e-3	4.75e-2	1.32
	1/256	8.58e-1	6.62e-2	1.20e-2	1.92

Table 3: Numerical results originated from the application of EF-standard and EF-revised SDIRK method with two-stages and order 2, to problem (6.22) for different values of the parameter λ and of the stepsize h. err^S, cd^S, err^R and cd^R denote the global error and the number of gained correct digits for the standard and the revised EF-based methods, respectively

λ	h	err^S	cd^S	err^R	cd^R
-1	1/16	5.01e-4	3.30	3.99e-4	3.40
	1/32	1.24e-4	3.90	1.05e-4	3.98
	1/64	3.11e-5	4.51	2.70e-5	4.57
	1/128	7.77e-6	5.11	6.84e-6	5.16
-2	1/16	8.81e-4	3.05	2.22e-5	4.65
	1/32	2.15e-4	3.67	5.37e-6	5.27
	1/64	5.31e-5	4.27	1.31e-6	5.88
	1/128	1.32e-5	4.88	3.25e-7	6.49
-4	1/16	2.00e-3	2.70	6.32e-7	6.20
	1/32	4.74e-4	3.32	1.67e-7	6.78
	1/64	1.15e-4	3.94	4.27e-8	7.37
	1/128	2.85e-5	4.54	1.08e-8	7.97

Table 4: Numerical results originated from the application of EF-standard and EF-revised SDIRK method with two-stages and order 2, to problem (6.23) for different values of the parameter λ and of the stepsize h. err^S, cd^S, err^R and cd^R denote the global error and the number of gained correct digits for the standard and the revised EF-based methods, respectively

ones becomes more visible the more the problem exhibits a prominent exponential behaviour. Anyway, we are aware of the fact that the price to be paid for the increased accuracy of the revised formula is the evaluation of the Jacobian of the vector field for the computation of the coefficients of the method. In order to avoid further function evaluations due to the computation of the coefficients of the revised EF-methods, we aim to suitably approximate the partial derivatives that appear in the coefficients of the revised formula, by means of numerical differentiation formulae whose accuracy is coherent with the expected order of convergence of the overall numerical scheme. This topic will be object of future research.

Acknowledgments

The authors wish to thank Prof. Liviu Gr. Ixaru for the profitable and inspiring discussions had on the topic. We also express our gratitude to the anonymous referees for their profitable comments.

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