Exponentially fitted two-step hybrid methods for $y'' = f(x, y)$

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Abstract

It is the purpose of this paper to derive two-step hybrid methods for $y'' = f(x, y)$, with oscillatory or periodic solutions, specially tuned to the behaviour of the solution, through the usage of the exponential fitting technique. The construction of two-step exponentially fitted hybrid methods is shown and their properties are discussed. Some numerical experiments confirming the theoretical expectations are provided.

Keywords: Second order ordinary differential equations, two-step hybrid methods, exponential fitting.

1. Introduction

It is the purpose of this paper to derive numerical methods approximating the solution of initial value problems based on second order ordinary differential equations (ODEs)

$$\begin{cases} y'' = f(x, y), \\ y'(x_0) = y'_0, \\ y(x_0) = y_0, \end{cases} \tag{1.1}$$

with $f : [x_0, X] \times \mathbb{R}^d \to \mathbb{R}^d$ smooth enough in order to ensure the existence and uniqueness of the solution, which is assumed to exhibit a periodic/oscillatory behaviour. Although the problem (1.1) could be transformed into a doubled dimensional system of first order ODEs and solved by standard formulae for first order differential systems, the development of numerical methods for its direct integration seems more natural and efficient.

Second order ODEs (1.1) having periodic or oscillatory solutions often appear in many applications, e.g. celestial mechanics, seismology, molecular dynamics, and so on (see for instance [24, 31] and references therein contained). Classical numerical methods for ODEs may not be well-suited to follow a prominent periodic or oscillatory behaviour because, in order to accurately catch the oscillations, a very small stepsize would be required with corresponding deterioration of the numerical performances, especially in terms of efficiency. For this reason, many classical numerical methods have been adapted in order to efficiently approach the oscillatory behaviour. One of the possible ways to proceed in this direction 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 technique (EF, see [18]), where the adapted numerical method is developed in order to be exact on problems whose solution is linear combination of

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

where K and P are integer numbers.

In the context of linear multistep methods for second order ODEs, Gautschi [13] and Stiefel-Bettis [28] considered trigonometric functions depending on one or more frequencies, while Lyche [20] derived methods exactly integrating initial value problems based on ODEs of order r whose solution can be expressed as linear combination of powers and exponentials; Raptis-Allison [26] and Ixaru-Rizea [16] derived special purpose linear multistep methods for the numerical treatment of the radial Schrödinger equation $y'' = (V(x) - E)y$, by means of trigonometric and exponential basis of functions. More recently, in the context of Runge–Kutta–Nyström methods, exponentially-fitted methods have been considered, for instance, by Calvo [3], Franco [12], Simos [1, 27] and Vanden Berghe [29], while their trigonometrically-fitted version has been developed by Paternoster in [21]; mixed-collocation based Runge–Kutta–Nyström methods have been introduced by Coleman and Duxbury in [5]. Recent adaptations of the Numerov method have been provided in [11, 14, 30]. For a more extensive bibliography see [18] and references within.

The methods we consider in this paper belong to the class of two-step hybrid methods

$$Y_i^{[n]} = (1 + c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i = 1, ..., s \tag{1.2}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(Y_i^{[n]}), \tag{1.3}$$

introduced by Coleman in [4], which can also be represented through the Butcher array

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \tag{1.4}$$

with $c = [c_1, c_2, ..., c_s]^T$, $A = (a_{ij})_{i,j=1}^s$, $b = [b_1, b_2, ..., b_s]^T$, where s is the number of stages. The interest in this class of methods, as also pointed out by Coleman in [4], lies in their formulation: “many other methods, though not normally written like this, can be expressed in the same way by simple rearrangement”. For this reason, they represent one of the first attempts to obtain wider and more general classes of numerical methods for (1.1), towards a class of General Linear Methods [2, 7, 10, 19] for this problem.

The aim of this paper is the derivation of EF-based methods within the class (1.2)-(1.3) depending on one or two parameters, which we suppose can be estimated in advance. Frequency-dependent methods within the class (1.2)-(1.3) have already been considered in [33], where phase-fitted and amplification-fitted two-step hybrid methods have been derived, and also in [9], where trigonometrically fitted methods (1.2)-(1.3) depending on one and two frequencies have been proposed.

In Section 2 we present the constructive technique of EF methods of type (1.2)-(1.3). Section 3 is devoted to the local error analysis and the parameter estimation, while in Section 4 we analyze the linear stability properties of the derived methods. Finally section 5 provides numerical tests confirming the theoretical expectations. The paper concludes with an appendix, where some examples of methods have been reported.

2. Construction of the methods

We present the constructive technique we used to derive EF methods within the class (1.2)-(1.3), based on the so-called six-step procedure, introduced by Ixaru and Vanden Berghe in [18] as a constructive tool to derive EF based formulae approaching many problems of Numerical Analysis (e.g. interpolation, numerical quadrature and differentiation, numerical solution of ODEs) especially when their solutions show a prominent periodic/oscillatory behaviour. This procedure provides a general way to derive EF formulae whose coefficients are expressed in a regularized way and, as a consequence, they do not suffer from numerical cancellation. Indeed, coefficients expressed as linear combinations of sine, cosine and exponentials suffer from heavy numerical cancellation and, in the implementation, they are generally replaced by their power series expansion, suitably truncated. On the contrary, the coefficients of EF methods obtained by using the six-step flow chart are expressed by means of the $\eta_k(s)$ functions introduced by Ixaru (see [15, 18] and references therein contained) and, as a consequence, the effects of numerical cancellation are notably reduced.

In agreement with the procedure, we first consider the following set of $s + 1$ functional operators

$$\mathcal{L}[h, \mathbf{b}]y(x) = y(x + h) - 2y(x) + y(x - h) - h^2 \sum_{i=1}^{s} b_i y''(x + c_i h), \tag{2.1}$$

$$\mathcal{L}_i[h, \mathbf{a}]y(x) = y(x + c_i h) - (1 + c_i)y(x) + c_i y(x - h) - h^2 \sum_{j=1}^{s} a_{ij} y''(x + c_j h), \; i = 1, \dots, s, \tag{2.2}$$

which are associated to the method (1.2)-(1.3). We next report the first five steps of the procedure, while the remaining one, i.e. the local error analysis, is reported in Section 3.

- step (i) *Computation of the classical moments*. The reduced classical moments (see [18], p. 42) are defined, in our case, as

$$L^*_{im}(\mathbf{a}) = h^{-(m+1)}\mathcal{L}_i[h;\mathbf{a}]x^m,\ i=1,\dots,s,\ m=0,1,2,\dots, \tag{2.3}$$
$$L^*_{m}(\mathbf{b}) = h^{-(m+1)}\mathcal{L}[h;\mathbf{b}]x^m,\ m=0,1,2,\dots \tag{2.4}$$

- step (ii) *Compatibility analysis*. We examine the algebraic systems

$$L^*_{im}(\mathbf{a}) = 0,\ i=1,\dots,s,\ m=0,1,\dots,M-1, \tag{2.5}$$
$$L^*_{m}(\mathbf{b}) = 0,\ m=0,1,\dots,M'-1, \tag{2.6}$$

to find out the maximal values of M and M' for which the above systems are compatible. If $s=2$, we have

$$\begin{array}{lll}
L^*_0 = 0, & L^*_{10} = 0, & L^*_{20} = 0,\\
L^*_1 = 0, & L^*_{11} = 0, & L^*_{21} = 0,\\
L^*_2 = 2(1-b_1-b_2), & L^*_{12} = c_1 + c_1^2 - 2(a_{11}+a_{12}), & L^*_{22} = c_2 + c_2^2 - 2(a_{21}+a_{22}),\\
L^*_3 = 6(-b_1c_1 - b_2c_2), & L^*_{13} = -c_1(1+6a_{11}-c_1^2) - 6a_{12}c_2, & L^*_{23} = -c_2(1+6a_{22}-c_2^2) - 6a_{21}c_1,\\
L^*_4 = 12(\frac{1}{6} - b_1c_1^2 - b_2c_2^2), & L^*_{14} = c_1 + c_1^4 - 12(a_{11}c_1^2 + a_{12}c_2^2), & L^*_{24} = c_2 + c_2^4 - 12(a_{21}c_1^2 + a_{22}c_2^2),
\end{array}$$

and, therefore, $M = M' = 4$.

- step (iii) *Computation of the G functions*. In order to derive EF methods, we need to compute the so-called *reduced (or starred) exponential moments* (see [18], p. 42), i.e.

$$E^*_{0i}(\pm z,\mathbf{a}) = \exp(\pm\mu x)\mathcal{L}_i[h,\mathbf{a}]\exp(\pm\mu x), i=1,\dots,s, \tag{2.7}$$
$$E^*_{0}(\pm z,\mathbf{b}) = \exp(\pm\mu x)\mathcal{L}[h,\mathbf{b}]\exp(\pm\mu x), \tag{2.8}$$

where $z=\mu h$. Once computed the reduced exponential moments, we can derive the G functions, defined in the following way:

$$G_i^+(Z,\mathbf{a}) = \frac{1}{2}\Big(E^*_{0i}(z,\mathbf{a}) + E^*_{0i}(-z,\mathbf{a})\Big),\quad i=1,\dots,s,$$
$$G_i^-(Z,\mathbf{a}) = \frac{1}{2z}\Big(E^*_{0i}(z,\mathbf{a}) - E^*_{0i}(-z,\mathbf{a})\Big),\quad i=1,\dots,s,$$
$$G^+(Z,\mathbf{b}) = \frac{1}{2}\Big(E^*_{0}(z,\mathbf{b}) + E^*_{0}(-z,\mathbf{b})\Big),$$
$$G^-(Z,\mathbf{b}) = \frac{1}{2z}\Big(E^*_{0}(z,\mathbf{b}) - E^*_{0}(-z,\mathbf{b})\Big),$$

where $Z=z^2$. In our case, the G functions take the following form

$$G_i^+(Z,\mathbf{a}) = \eta_{-1}(c_i^2Z) + c_i\eta_{-1}(Z) - 2(1+c_i) - Z\sum_{j=1}^{s} a_{ij}\eta_{-1}(c_j^2Z),\quad i=1,\dots,s,$$
$$G_i^-(Z,\mathbf{a}) = c_i\eta_0(c_i^2Z) - c_i\eta_0(Z) - 2(1+c_i) - Z\sum_{j=1}^{s} c_ja_{ij}\eta_0(c_j^2Z),\quad i=1,\dots,s,$$
$$G^+(Z,\mathbf{b}) = 2\eta_{-1}(Z) - 2 - Z\sum_{j=1}^{s} b_j\eta_{-1}(c_j^2Z),$$
$$G^-(Z,\mathbf{b}) = -Z\sum_{j=1}^{s} b_jc_j\eta_0(c_j^2Z).$$

We observe that the above expressions depend on the functions $\eta_{-1}(Z)$ and $\eta_0(Z)$ (compare [15, 18]), which are defined as follows

$$\eta_{-1}(Z) = \frac{1}{2}[\exp(Z^{1/2}) + \exp(-Z^{1/2})] = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \le 0, \\ \cosh(Z^{1/2}) & \text{if } Z > 0, \end{cases}$$

and

$$\eta_0(Z) = \begin{cases} \dfrac{1}{2Z^{1/2}}[\exp(Z^{1/2}) - \exp(-Z^{1/2})] & \text{if } Z \ne 0, \\ 1 & \text{if } Z = 0, \end{cases} = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0, \\ 1 & \text{if } Z = 0, \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0. \end{cases}$$

We next compute the p-th derivatives $G^{\pm(p)}$ and $G_i^{\pm(p)}$, taking into account the formula for the p-th derivative of $\eta_k(Z)$ (see [18]), i.e.

$$\eta_k^{(p)}(Z) = \frac{1}{2^p}\eta_{k+p}(Z).$$

We thus obtain

$$\begin{aligned}
G_i^{+(p)}(Z, \mathbf{a}) &= \frac{c_i^{2p}}{2^p}\eta_{p-1}(c_i^2 Z) + \frac{c_i}{2^p}\eta_{p-1}(Z) - \sum_{j=1}^{s} a_{ij}\frac{d^p}{dZ^p}\Big(Z\eta_{-1}(c_j^2 Z)\Big), \quad i = 1, \ldots, s, \\
G_i^{-(p)}(Z, \mathbf{a}) &= \frac{c_i^{2p+1}}{2^p}\eta_p(c_i^2 Z) - \frac{c_i}{2^p}\eta_p(Z) - \sum_{j=1}^{s} a_{ij}c_j\frac{d^p}{dZ^p}\Big(Z\eta_0(c_j^2 Z)\Big), \quad i = 1, \ldots, s, \\
G^{+(p)}(Z, \mathbf{b}) &= \frac{1}{2^{p-1}}\eta_{p-1}(Z) - \sum_{j=1}^{s} b_j\frac{d^p}{dZ^p}\Big(Z\eta_{-1}(c_j^2 Z)\Big), \\
G^{-(p)}(Z, \mathbf{b}) &= -\sum_{j=1}^{s} b_j c_j\frac{d^p}{dZ^p}\Big(Z\eta_{-1}(c_j^2 Z)\Big).
\end{aligned}$$

- step (iv) *Definition of the function basis*. We next decide the shape of the function basis to take into account: as a consequence, the corresponding method will exactly integrate (i.e. the operator $\mathcal{L}[h, \mathbf{b}]y(x)$ annihilates in correspondence of the function basis) all those problems whose solution is linear combination of the basis functions. In general, the set of M functions is a collection of both powers and exponentials, i.e.

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

  where K and P are integer numbers satisfying the relation

  $$K + 2P = M - 3. \tag{2.9}$$

  Let us next consider the set of M' functions

  $$\{1, x, \ldots, x^{K'}, \exp(\pm\mu x), x\exp(\pm\mu x), \ldots, x^{P'}\exp(\pm\mu x)\} \tag{2.10}$$

  annihilating the operators $\mathcal{L}_i[h, \mathbf{a}]y(x)$, $i = 1, 2, \ldots, s$ and assume that $K' = K$ and $P' = P$, i.e. the external stage and the internal ones are exact on the same function basis. We observe that other possible choices can be taken into account: this can be explained by means of the compatibility of the linear systems to be solved in order to derive the parameters of the methods. In fact, the s^2 unknown elements of the matrix A are derived by solving a linear system of $s(K' + 2P' + 3)$ equations, while the s elements of the vector b are the solution of a $K + 2P + 3$ dimensional linear system. Such systems are compatible if and only if

  $$\begin{cases} s^2 = s(K' + 2P' + 3), \\ s = K + 2P + 3, \end{cases}$$

or, equivalently, if $K' + 2P' = K + 2P$. One natural choice which satisfies this requirement is, of course, $K' = K$ and $P' = P$, but other possibilities can be certainly taken into account, even if they are not explored in this paper.

- step (v) *Determination of the coefficients*. After a suitable choice of K and P, we next solve the following algebraic systems:

$$G_i^{\pm(p)}(Z, \mathbf{a}) = 0,\ i = 1, \dots, s,\ p = 0, ..., P,$$
$$G^{\pm(p)}(Z, \mathbf{b}) = 0,\ p = 0, ..., P.$$

The paper focuses on the complete analysis of two-stage EF methods with $K = -1$ and $P = 1$ within the class (1.2)-(1.3), whose coefficients have been reported in the appendix. In correspondence to this choice of K and P, the fitting space assumes the form

$$\{1, x, \exp(\pm\mu x), x\exp(\pm\mu x)\}. \tag{2.11}$$

We observe that, even if $K = -1$, the monomial x is present in the basis (2.11), because it automatically annihilates the linear operators (2.1)-(2.2).

It is also possible to extend the above procedure in order to derive EF methods belonging to the class (1.2)-(1.3), in the case of more than one parameter. In particular, the appendix reports the coefficients of two-parameters EF methods with 4 stages, with respect to the basis of functions

$$\{1, x, \exp(\pm\mu_1 x), \exp(\pm\mu_2 x)\}. \tag{2.12}$$

The final step of this procedure, i.e. the error analysis of the derived formulae, is reported in Section 3.

3. Error analysis and estimation of the parameters

According to the used procedure, the general expression of the local truncation error for an EF method with respect to the basis of functions (2.10) takes the form (see [18])

$$lte^{EF}(x) = (-1)^{P+1} h^M \frac{L^*_{K+1}(\mathbf{b}(Z))}{(K+1)! Z^{P+1}} D^{K+1}(D^2 - \mu^2)^{P+1} y(x), \tag{3.1}$$

with K, P and M satisfying the condition (2.9). Taking into account our choice (2.11) for the functional basis, we obtain

$$lte^{EF}(x) = \frac{L^*_2(\mathbf{b}(Z))}{2\mu^4} D^2(D^2 - \mu^2)^2 y(x). \tag{3.2}$$

We next expand lte^{EF} in Taylor series around x, evaluate it in the current point x_n and consider the leading term of the series expansion, obtaining

$$lte^{EF}(x_n) = -\frac{1 + 6c_1c_2}{24\mu^2} \left(\mu^4 y^{(2)}(x_n) - 2\mu^2 y^{(4)}(x_n) + y^{(6)}(x_n)\right) h^4 + O(h^5). \tag{3.3}$$

The local error analysis also constitutes a starting point for the estimation of the unknown parameter μ which is, in general, a nontrivial problem. In fact, up to now, a rigorous theory for the exact computation of the parameter μ has not yet been developed, but several attempts have been done in the literature in order to provide an accurate estimation (see [17, 18] and references therein), generally based on the minimization of the leading term of the local discretization error. For this reason we annihilate the term $\mu^4 y^{(2)}(x_n) - 2\mu^2 y^{(4)}(x_n) + y^{(6)}(x_n)$ and estimate the parameter in the following way:

$$\mu = \sqrt{\frac{y^{(4)}(x_n) + \sqrt{y^{(4)}(x_n)^2 - y''(x_n) y^{(6)}(x_n)}}{y''(x_n)}}. \tag{3.4}$$

The expressions for the occurring derivatives can be obtained analytically from the given ODEs (1.1).

4. Linear stability analysis

We next analyze the linear stability properties [6, 31, 32] of the resulting methods, taking into account their dependency on the parameters. The following definitions regard both the case of constant coefficients methods (1.2)-(1.3), and their exponentially fitted version.

4.1. Methods with constant coefficients

Following [31], we apply (1.2)-(1.3), to the test problem

$$y'' = -\lambda^2 y, \qquad \lambda \in \mathbb{R}$$

obtaining the following recurrence relation (see [8])

$$\begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix} = \begin{bmatrix} M_{11}(\nu^2) & M_{12}(\nu^2) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_n \\ y_{n-1} \end{bmatrix}, \tag{4.1}$$

where

$$M_{11}(\nu^2) = 2 - \nu^2 b^T Q(\nu^2)(e + c),$$
$$M_{12}(\nu^2) = -1 + \nu^2 b^T Q(\nu^2)c,$$

and $Q(\nu^2) = (I + \nu^2 A)^{-1}$, with $\nu^2 = h^2\lambda^2$. The matrix

$$M(\nu^2) = \begin{bmatrix} M_{11}(\nu^2) & M_{12}(\nu^2) \\ 1 & 0 \end{bmatrix}, \tag{4.2}$$

is the so-called *stability (or amplification) matrix* [31, 32]. Let us denote its spectral radius by $\rho(M(\nu^2))$. From [31, 32], the following definitions hold.

Definition 4.1. $(0, \beta^2)$ *is a stability interval for the method* (1.2)-(1.3) *if,* $\forall \nu^2 \in (0, \beta^2)$*, it is*

$$\rho(M(\nu^2)) < 1. \tag{4.3}$$

The condition (4.3) means that both the eigenvalues $\lambda_1(\nu^2)$ and $\lambda_2(\nu^2)$ of $M(\nu^2)$ are in modulus less than 1, $\forall \nu^2 \in (0, \beta^2)$. By setting $S(\nu^2) = \mathrm{Tr}(M^2(\nu^2))$ and $P(\nu^2) = \det(M^2(\nu^2))$, (4.3) is equivalent to

$$P(\nu^2) < 1, \quad |S(\nu^2)| < P(\nu^2) + 1, \quad \nu^2 \in (0, \beta^2). \tag{4.4}$$

Definition 4.2. *The method* (1.2)-(1.3) *is P-stable if* $(0, \beta^2) = (0, +\infty)$.

If $\lambda_1(\nu^2)$ and $\lambda_2(\nu^2)$ both lie on the unit circle, then the interval of stability becomes an interval of periodicity, according to the following definition.

Definition 4.3. $(0, H_0^2)$ *is a periodicity interval if,* $\forall \nu^2 \in (0, H_0^2)$*,* $\lambda_1(\nu^2)$ *and* $\lambda_2(\nu^2)$ *are complex conjugate and have modulus 1.*

Equivalently,

$$P(\nu^2) = 1, \quad |S(\nu^2)| < 2, \quad \forall \nu^2 \in (0, H_0^2). \tag{4.5}$$

Definition 4.4. *The method* (1.2)-(1.3) *is P-stable if its periodicity interval is* $(0, +\infty)$.

4.2. Methods depending on one and two frequencies

Coleman and Ixaru discussed in [6] the modifications to introduce in the linear stability analysis for one-parameter depending EF methods. As a consequence of the presence of the parameter μ, the interval of stability becomes a bidimensional stability region for the one parameter family of methods. In order to emphasize the dependency on the fitted parameter $Z = z^2$, we use the notation $M(\nu^2, Z)$, $R(\nu^2, Z) = \frac{1}{2}\mathrm{Tr}(M(\nu^2, Z))$, $P(\nu^2, Z) = \det(M(\nu^2, Z))$ to denote the stability matrix, its halved trace and determinant respectively. The following definition arises:

Definition 4.5. *A region of stability Ω is a region of the (ν^2, Z) plane, such that $\forall(\nu^2, Z) \in \Omega$*

$$P(\nu^2, Z) < 1, \quad |R(\nu^2, Z)| < (P(\nu^2, Z) + 1). \tag{4.6}$$

Any closed curve defined by $P(\nu^2, Z) \equiv 1$ and $|R(\nu^2, Z)| = \frac{1}{2}(P(\nu^2, Z) + 1)$ is a stability boundary.

We next consider the linear stability analysis of methods depending on two frequencies. As stated before, for methods with constant coefficients, the stability region is an interval on the real axis, while methods depending on one frequency have a bidimensional stability region. In the case of methods depending on the values of two parameters μ_1, μ_2 the stability region becomes tridimensional. We now denote the stability matrix of the methods as $M(\nu^2, Z_1, Z_2)$, with $Z_1 = \mu_1^2 h^2$ and $Z_2 = \mu_2^2 h^2$. The definition of stability region for two-parameters depending methods can be adapted as follows [8, 11]:

Definition 4.6. *A three dimensional region Ω of the (ν^2, Z_1, Z_2) space is said to be the region of stability of the corresponding two-frequency depending method if, $\forall(\nu^2, Z_1, Z_2) \in \Omega$,*

$$P(\nu^2, Z_1, Z_2) < 1, \quad |R(\nu^2, Z_1, Z_2)| < \frac{1}{2}(P(\nu^2, Z_1, Z_2) + 1). \tag{4.7}$$

Any closed curve defined by

$$P(\nu^2, Z_1, Z_2) \equiv 1, \quad |R(\nu^2, Z_1, Z_2)| = \frac{1}{2}(P(\nu^2, Z_1, Z_2) + 1). \tag{4.8}$$

is a stability boundary for the method.

Examples of bidimensional and tridimensional stability regions are provided in the appendix.

5. Numerical results

We now perform some numerical experiments confirming the theoretical expectations regarding the methods we have derived. The implemented solvers are based on the following methods:

- COLEM2, two-step hybrid method (1.2)-(1.3) having constant coefficients (see [8])

$$\begin{array}{c|cc} \frac{1}{2} & -1 & \\ 1 & 2 & -1 \\ \hline & 2 & -1 \end{array} \tag{5.1}$$

  with $s = 2$ and order 2;

- EXPCOLEM2, one-parameter depending exponentially-fitted method (1.2)-(1.3), with $s = 2$ and order 2, whose coefficients are reported in the appendix.

We implement such methods in a fixed stepsize environment, with step $h = \frac{1}{2^k}$, with k positive integer number. The numerical evidence confirms that EF-based methods within the class (1.2)-(1.3) are able to exactly integrate, within round-off error, problems whose solution is linear combination of the considered basis functions. This result also holds for large values of the stepsize: on the contrary, for the same values of the step of integration, classical methods (1.2)-(1.3) are less accurate and efficient, because in order to accurately integrate problems with oscillating solutions, classical methods require a very small stepsize, deteriorating the numerical performances in terms of efficiency.

Problem 1. We consider the following simple test equation

$$\begin{cases} y''(x) = \lambda^2 y(x), \\ y(0) = 1, \\ y'(0) = -\lambda, \end{cases} \tag{5.2}$$

with $\lambda > 0$ and $x \in [0, 1]$. The exact solution of this equation is $y(x) = \exp(-\lambda x)$ and, therefore, our exponentially-fitted methods can exactly reproduce it, i.e. the numerical solution will be affected by the round-off error only. Table 1 shows the results we have obtained by using the above numerical methods.

λ	k	COLEM2	EXPCOLEM2
2	4	8.32e-1	1.09e-14
	5	2.29e-1	3.94e-14
	6	5.96e-2	1.20e-13
3	7	2.71e-1	1.06e-12
	8	6.85e-2	7.96e-12
	9	1.72e-2	5.97e-12
4	8	9.09e-1	1.83e-11
	9	2.29e-1	2.26e-11
	10	5.74e-2	1.64e-10

Table 1: Relative errors corresponding to the solution of the problem (5.2), for different values of λ and k.

Problem 2. We examine the following linear equation

$$\begin{cases} y''(x) - y(x) = x - 1, \\ y(0) = 2, \\ y'(0) = -2, \end{cases} \tag{5.3}$$

with $\lambda > 0$ and $x \in [0, 5]$. The exact solution is $y(x) = 1 - x + \exp(-x)$ and, therefore, it is linear combinations of all the basis functions in (2.11). The obtained results are reported in Table 2.

k	COLEM2	EXPCOLEM2
5	8.53e-1	1.65e-14
6	2.71e-1	5.16e-14
7	7.26e-2	2.21e-13

Table 2: Relative errors corresponding to the solution of the problem (5.3).

Problem 3. We next focus on the Prothero-Robinson problem [25]

$$\begin{cases} y''(x) + \nu^2[y(x) - \exp(-\lambda x)]^3 = \lambda^2 y, \\ y(0) = 1, \\ y'(0) = -\lambda, \end{cases} \tag{5.4}$$

in $x \in [0, 5]$, which is a nonlinear problem whose exact solution is $y(x) = \exp(-\lambda x)$. The obtained results are reported in Table 3.

k	COLEM2	EXPCOLEM2
1	3.65e-1	2.41e-15
2	1.70e-1	3.16e-16
3	2.65e-2	1.21e-15

Table 3: Relative errors corresponding to the solution of the problem (5.4), with $\nu = 1/10$.

6. Conclusions and further developments

We have derived the exponentially-fitted version of the two-step hybrid methods introduced by Coleman in [4]. These methods take advantage from the knowledge of the qualitative behaviour of the solution, which is supposed to be of exponential type, depending on one or two parameters. The construction of the new formulae has been provided, together with the stability analysis, the computation of the local error and the estimation of the unknown parameters. Some numerical experiments have also been provided in order to confirm the theoretical expectations.

Future work will address the construction and the analysis of wider and more general classes of numerical methods for second order problems (1.1), falling in the class of General Linear Methods [2, 7, 10, 19, 22, 23].

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Appendix: some examples of methods

We report the coefficients of EF methods (1.2)-(1.3) with $s = 2$ and $s = 4$ with respect to the basis (2.11) and (2.12) respectively.

Two-stage EF methods within the class (1.2)-(1.3) and exact on the functional basis (2.11) have the following coefficients:

$$b_1 = -\frac{2c_2\left(\eta_{-1}(Z)-1\right)\eta_0\left(c_2^2 Z\right)}{Z\left(c_1\eta_0\left(c_1^2 Z\right)\eta_{-1}\left(c_2^2 Z\right) - c_2\eta_{-1}\left(c_1^2 Z\right)\eta_0\left(c_2^2 Z\right)\right)},$$

$$b_2 = \frac{2c_1\left(\eta_{-1}(Z)-1\right)\eta_0\left(c_1^2 Z\right)}{Z\left(c_1\eta_0\left(c_1^2 Z\right)\eta_{-1}\left(c_2^2 Z\right) - c_2\eta_{-1}\left(c_1^2 Z\right)\eta_0\left(c_2^2 Z\right)\right)},$$

$$a_{11} = \frac{-c_2\eta_{-1}\left(c_1^2 Z\right) + c_1\eta_0\left(c_1^2 Z\right) - c_1c_2\eta_{-1}(Z) + 2c_1c_2 - c_1\eta_0(Z) - 2c_1 + 2c_2 - 2}{Z(c_1-c_2)\eta_{-1}\left(c_1^2 Z\right)},$$

$$a_{12} = \frac{c_1^2\eta_{-1}(Z) + c_1\eta_{-1}\left(c_1^2 Z\right) - c_1\eta_0\left(c_1^2 Z\right) - 2c_1^2 + c_1\eta_0(Z) + 2}{Z(c_1-c_2)\eta_{-1}\left(c_2^2 Z\right)},$$

$$a_{21} = \frac{c_2^2\left(-\eta_{-1}(Z)\right) - c_2\eta_{-1}\left(c_2^2 Z\right) + c_2\eta_0\left(c_2^2 Z\right) + 2c_2^2 - c_2\eta_0(Z) - 2}{Z(c_1-c_2)\eta_{-1}\left(c_1^2 Z\right)},$$

$$a_{22} = \frac{c_1\eta_{-1}\left(c_2^2 Z\right) + c_1c_2\eta_{-1}(Z) - 2c_1c_2 - 2c_1 - c_2\eta_0\left(c_2^2 Z\right) + c_2\eta_0(Z) + 2c_2 + 2}{Z(c_1 - c_2)\eta_{-1}\left(c_2^2 Z\right)}.$$

It is easy to prove that, for Z tending to 0, these coefficients tend to those of two-step hybrid methods based on algebraic collocation (see [8]): therefore, applying the order conditions derived in [4] for Z tending to 0, we discover that these methods have order 2. Fig. 1 shows an example of stability region for two-stage one-parameter depending method with $c_1 = \frac{2}{3}$, $c_2 = \frac{4}{5}$.

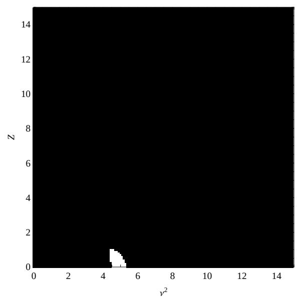

Figure 1: Region of stability in the $(v^2, Z)-$plane for $s = 2$, with $c_1 = \frac{2}{3}$, $c_2 = \frac{4}{5}$.

The coefficients of four-stage EF methods (1.2)-(1.3) with respect to the functional basis (2.12) are too long to be reported in the paper and, for this reason, we present their truncated power series expansion, in correspondence of the abscissa vector $c = [0, \frac{1}{3}, \frac{2}{3}, 1]^T$:

$$\begin{aligned}
b_1 &= \frac{5}{2} + \frac{43\,{Z_2}^2}{360} + \left(\frac{43}{360} + \frac{593\,{Z_2}^2}{272160}\right){Z_1}^2 + O(Z_1^4) + O(Z_2^4),\\
b_2 &= -\frac{15}{4} - \frac{37\,{Z_2}^2}{144} - \left(\frac{37}{144} + \frac{9643\,{Z_2}^2}{544320}\right){Z_1}^2 + O(Z_1^4) + O(Z_2^4),\\
b_3 &= 3 + \frac{7\,{Z_2}^2}{45} + \left(\frac{7}{45} + \frac{593\,{Z_2}^2}{136080}\right){Z_1}^2 + O(Z_1^4) + O(Z_2^4),\\
b_4 &= -\frac{3}{4} - \frac{13\,{Z_2}^2}{720} - \left(\frac{13}{720} + \frac{47\,{Z_2}^2}{544320}\right){Z_1}^2 + O(Z_1^4) + O(Z_2^4),\\
a_{11} &= 0, \qquad a_{12} = 0, \qquad a_{13} = 0, \qquad a_{14} = 0,\\
a_{21} &= \frac{67}{81} + \frac{581Z_2^2}{14580} + \left(\frac{581}{14580} + \frac{24001Z_2^2}{33067440}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),\\
a_{22} &= -\frac{71}{54} - \frac{833Z_2^2}{9720} + \left(-\frac{833}{9720} - \frac{18607Z_2^2}{3149280}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),\\
a_{23} &= \frac{26}{27} + \frac{7Z_2^2}{135} + \left(\frac{7}{135} + \frac{533Z_2^2}{367416}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),\\
a_{24} &= -\frac{41}{162} - \frac{35Z_2^2}{5832} + \left(-\frac{35}{5832} - \frac{1919Z_2^2}{66134880}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),\\
a_{31} &= \frac{539}{324} + \frac{929Z_2^2}{11664} + \left(\frac{929}{11664} + \frac{27443Z_2^2}{18895680}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),
\end{aligned}$$

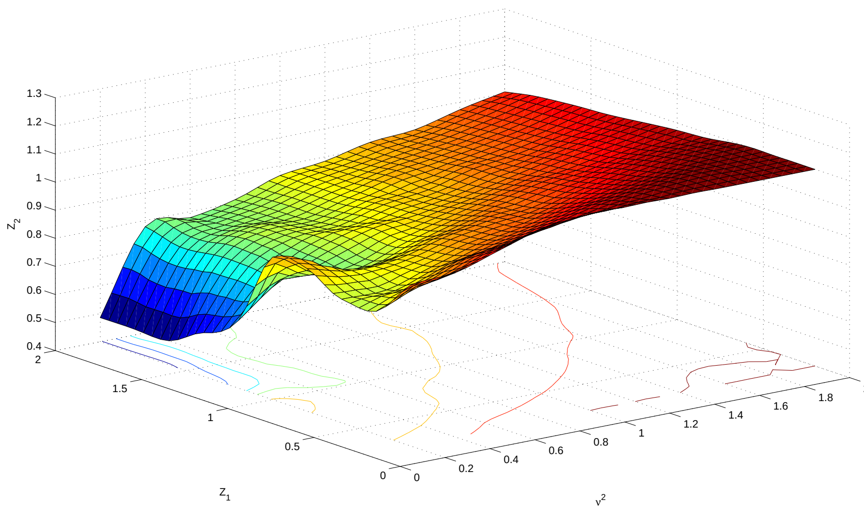

Figure 2: Region of stability in the (v^2, Z_1, Z_2)-space for $s = 4$, with $c = [0, \frac{1}{3}, \frac{2}{3}, 1]^T$.

$$a_{32} = -\frac{137}{54} - \frac{37Z_2^2}{216}\left(-\frac{37}{216} - \frac{86801Z_2^2}{7348320}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),$$

$$a_{33} = \frac{209}{108} + \frac{403Z_2^2}{3888} + \left(\frac{403}{3888} + \frac{127951Z_2^2}{44089920} +\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),$$

$$a_{34} = -\frac{41}{81} - \frac{35Z_2^2}{2916} + \left(-\frac{35}{2916} - \frac{1919Z_2^2}{33067440} +\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),$$

$$a_{41} = \frac{5}{2} + \frac{43Z_2^2}{360} + \left(\frac{43}{360} + \frac{593Z_2^2}{272160}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),$$

$$a_{42} = -\frac{15}{4} - \frac{37Z_2^2}{144} - \left(\frac{37}{144} + \frac{9643}{139860}Z_1^2\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),$$

$$a_{43} = 3 + \frac{7Z_2^2}{45} + \left(\frac{593Z_2^2}{136080} + \frac{7}{45}\right)Z_1^2 + O(Z_1^4) + O(Z_2^4),$$

$$a_{44} = -\frac{3}{4} - \frac{13Z_2^2}{720} - \left(\frac{13}{720} + \frac{47}{544320}Z_2^2\right)Z_1^2 + O(Z_1^4) + O(Z_2^4).$$

Also in this case, for Z_1 and Z_2 tending to 0, such coefficients tend to those of two-step hybrid methods based on algebraic collocation and the corresponding method has algebraic order 4. The tridimensional stability region of this method is reported in Fig. 2.

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