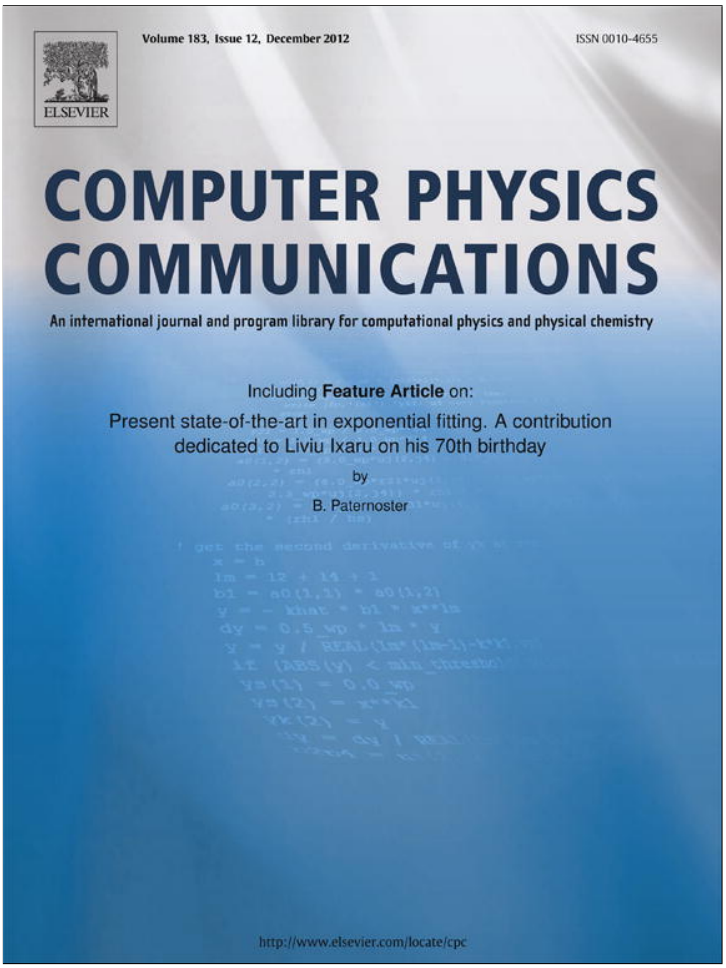

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Feature article

Present state-of-the-art in exponential fitting. A contribution dedicated to Liviu Ixaru on his 70th birthday

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ABSTRACT

The standard monograph in this area is the book *Exponential fitting* by Ixaru and Vanden Berghe (Kluwer, Boston - Dordrecht - London, 2004) but a fresh look on things is necessary because many new contributions have been accumulated in the meantime. With no claim that our investigation is exhaustive we consider various directions of interest, try to integrate the new contributions in a natural, easy to follow way, and also detect some open problems of acute interest.

1. Introduction

Exponential fitting is an area of flourishing interest in the last few decades, with hundreds of papers published in various journals on issues ranging from theory to applications. The only monograph on this field is the book of Ixaru and Vanden Berghe [1]. This book was published in 2004 but many important contributions have appeared in the meantime and then a fresh review to include the new achievements becomes appropriate.

Liviu Ixaru brought many valuable, seminal ideas which substantially helped in shaping the field, and this is why I want to dedicate this work to him, on his 70th birthday.

Liviu Ixaru was born on April 30, 1942 in Rascani-Balti (now in the Republic of Moldova) as the only child of a family of teachers. His primary and secondary school education was in Gaesti (a little town not far from Bucharest), where he was a brilliant pupil with largely diversified interests: literature, history, music (he was a gifted mandolin player), foreign languages (he is fluent in a few languages), and mathematics and physics, of course. His gift for the latter, gently guided by his father, a teacher of mathematics and physics in a secondary school, became obvious even in these years: his first paper (an extension of a theorem in classical geometry) was published just before he was 18, in a quite popular journal among young mathematicians in Romania [2].

In 1959 he became a student at the Faculty of Mathematics and Physics of the University of Bucharest and obtained in 1964 his master degree in Theoretical Physics, with a thesis on the shell model of the atomic nucleus under the guidance of Prof. Titeica. After a short intermezzo in the Institute of Physics of the Romanian Academy, in April 1965 he joined the department of Theoretical Physics of the Institute of Atomic Physics, where he continues to work today.

In his first active years (1965–1970) he was working on the theory of the spontaneous alpha decay of heavy nuclei. He investigated the influence of the internal structure of the alpha particle (until then this was taken as punctual) on the decay rates, and he has shown that this leads to a decrease of the rate, in accordance with the experimental evidence, see e.g. [3]. The activity during this investigation was crucial for shaping his method in the years to come. Since a serious numerical effort was needed, on one hand, and the computers available at that time were rather primitive (in Romania, at least), on the other hand, he soon understood that a significant progress in physics is impossible without developing new numerical methods to compensate for the weak equipment. In this way he became a pioneer of computational physics in that country, and his first result in this domain was a set of two papers, disseminated in 1969 as internal reports [4,5] but never published in regular journals, in which he formulated the embryo of what in the meantime became the successful CP methods for the Schrödinger equation. Subsequent progress in this direction (error analysis [6], improving the accuracy etc.) provided the basis of his Ph.D. thesis in theoretical physics (1973) under Prof. Corciovei, [7]. As for papers published in journals, see [8–13]. All these, and not only, were at the basis of Chapter 3 in Ixaru's book [14] which is the first systematic description of these methods and which is still today the main reference in this field. More recent advances include the formulation of a CP version of order 12 (at that time, this was the highest order reached by a numerical method), [15,16], extension to the 2D Schrödinger equation and a new formulation of the LP version, [17,18].

Liviu's first contact with the exponential fitting (ef) was in 1979. Shortly before, Raptis and Allison had published a paper, [19], based on Lyche's theory [20], where the famous Numerov method

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was adapted by exponential fitting to become tuned on the Schrödinger equation. Liviu realized that this version represents only the lowest level of adaptation and that two more, higher levels are available. The two new versions were presented in joint papers with Rizea, [21,22]. They convinced the readers that the exponential fitting is a very flexible approach and thus they produced a major momentum for the development of the whole field. Together with Coleman, Liviu has addressed two important theoretical issues. The first regards the stability properties of ef-based methods for differential equations, [23], and the stability function and stability regions, as defined by them, became fundamental concepts in any further investigation in this area. The second refers to the expression of the error for ef-based approximation formulae, [24]. In that paper they have shown that, in contrast to the classical approximation formulae, where the error has a Lagrange-like form, for ef-based formulae this is a sum of two such terms. This result is important not only from a theoretical but also from a practical point of view: it shows that the error estimates in terms of the leading term of the error (*lte*), as done quite often, are sometimes incorrect. In [25] Liviu addresses another important issue: how large is the class of approximations to be approached by the exponential fitting? He shows that the ef is appropriate not only for deriving tuned algorithms for differential equations but also for other numerical operations such as numerical differentiation, quadrature or interpolation. He introduced a general scheme to treat them, the so called six-step flow chart, which became popular in different contexts later on.

In all his activity Liviu has paid a special attention on having the theoretical results accompanied by ready-to-use codes, [14,1,26,27], and also on developing specific applications on hot problems. Thus, in a collaboration with Scott and Scott, [28], a special ef-based quadrature formula was built up for the computation of the Slater integrals. The new formula is by two orders of magnitude faster than the standard approach. This work has received the HPC prize (2006).

2. General remarks

The first acceptance which comes to mind for the expression 'exponential fitting' (ef) is that of a procedure intended to approximate a function through a linear combination of exponential functions. However, the actual object of this field is quite different: it is just assumed that the functions of interest are of the form

$$y(x) = \sum_{i=1}^{I} f_i(x) \exp(\mu_i x), \quad x \in [a, b] \tag{2.1}$$

and the object of the ef consists of producing algorithms for *operations* tuned on such functions as, for example, the numerical approach of differential equations with solution of this form, numerical differentiation, quadrature, interpolation of such functions etc. The weights $f_i(x)$ are assumed to vary slowly enough to be well approximated by low degree polynomials, and μ_i, called frequencies, are complex constants. As a matter of fact, the expression *exponential fitting* with the stated meaning seems to have been first used in the context of solving ODEs, by Liniger and Willoughby [29].

There is a huge practical interest in working on such functions because many phenomena are described in terms of these. The case of pure real and negative frequencies is essential in processes like decay, damping or absorbtion while pairs of imaginary conjugate frequencies are of help in describing oscillatory phenomena. For example, if $I = 2, f_1(x) = f_2(x)$ and $\mu_1 = i\omega$, $\mu_2 = -i\omega$ with real ω we have

$$y(x) = f_1(x)[\exp(i\omega x) + \exp(-i\omega x)] = 2f_1(x)\cos(\omega x).$$

Applications on problems involving oscillations, vibrations, rotations or wave propagation, in various branches of engineering and classical physics, or wavefunctions in quantum mechanics will then benefit directly from such a treatment.

Seen from a mathematical point of view, the case when $y(x)$ is a slowly varying function, which is the starting point when building up any classical algorithm (think, for example, of the multistep algorithms for differential equations or of the Newton–Cotes quadrature rules), is the particular case of (2.1) when all frequencies vanish. It is then natural to expect that the new algorithms, which depend on the frequencies, will tend to the classical ones when these frequencies tend to zero.

To understand the core of the procedure we take the standard case of the Numerov method. This is a two-step method for solving a second order ODE of form

$$y'' = f(x, y), \quad x \in [a, b], \tag{2.2}$$

where $f(x, y), f : \Re \times \Re^n \to \Re^n$. The algorithm is of the form

$$y_{n+1} + a_1 y_n + y_{n-1} = h^2[b_0(f_{n+1} + f_{n-1}) + b_1 f_n], \tag{2.3}$$

where h is the stepwidth, $x_{n\pm1} = x_n \pm h$, y_n is an approximation to $y(x_n)$ and $f_n = f(x_n, y_n)$. It allows obtaining y_{n+1} in terms of y_{n-1} and y_n (forward propagation) or y_{n-1} in terms of y_n and y_{n+1} (backwards propagation). If $f(x, y)$ is linear in y the computation of the new y_{n+1} or y_{n-1} is direct. Otherwise an iteration process is needed.

To determine the coefficients a_1, b_0, b_1, an operator representing the difference between the two sides of Eq. (2.3) is introduced,

$$\mathcal{L}[h, a_0, b_0, b_1]y(x) := y(x + h) + a_1 y(x) + y(x - h) - h^2[b_0(y''(x + h) + y''(x - h)) + b_1 y''(x)], \tag{2.4}$$

and it is required that $\mathcal{L}[h, a_0, b_0, b_1]y(x)$ vanishes when $y(x)$ belongs to a certain set of functions. If this is the power function set $y(x) = 1, x, x^2, \ldots$ then we get the classical coefficients $a_1 = -2, b_0 = 1/12, b_1 = 5/6$. It is easy to find out that $\mathcal{L}y$ with these coefficients is vanishing for the subset of $M = 6$ functions

$$y(x) = x^n, \quad n = 0, 1, \ldots, M - 1 = 5 \tag{2.5}$$

and for any linear combination of them, of course. Expressed in other words, the Numerov method with classical coefficients is exact when the solution $y(x)$ is a fifth degree polynomial.

A natural question is: can a set of M functions different from the power functions be used to build up the coefficients? Raptis and Allison have used

$$y(x) = x^k, \quad k = 0, 1, 2, 3, \exp(\pm\mu x) \tag{2.6}$$

where μ is either a real or a purely imaginary constant, and have obtained: $a_1 = -2$,

$$b_0(Z) = \begin{cases} \dfrac{1}{Z}\left[1 - \dfrac{Z}{4\sinh^2(\sqrt{|Z|}/2)}\right] & \text{if } Z > T \\ \dfrac{1}{12} - \dfrac{1}{240}Z + \dfrac{1}{6048}Z^2 - \dfrac{1}{172800}Z^3 + \dfrac{1}{5322240}Z^4 & \\ \quad \text{if } -T \le Z \le T & \\ \dfrac{1}{Z}\left[1 + \dfrac{Z}{4\sin^2(\sqrt{|Z|}/2)}\right] & \text{if } Z < -T \end{cases}$$

and $b_2(Z) = 1 - 2b_1(Z)$, where $Z = (\mu h)^2$ (notice that Z is real irrespective of whether μ is real or purely imaginary). T is a threshold value chosen in terms of the wordlength used; the value $T = 0.1$ is convenient for double precision computations.

This version is exact for $y(x) = f_1(x) + c_1 \sin(|\mu|x) + c_2 \cos(|\mu|x)$ or $y(x) = f_1(x) + c_1 \sinh(\mu x) + c_2 \cosh(\mu x)$, if μ is imaginary or real, respectively, where $f_1(x)$ is a third degree polynomial and c_1 and c_2 are constants. It has been built up for the Schrödinger equation, and extends the algorithm of Stiefel and Bettis [30] for the orbit

problem in celestial mechanics; the latter considered only the case of imaginary μ.

The idea of using a basis of functions other than polynomials has a long history, going back at least to the papers of Greenwood [31], Brock and Murray [32] and Dennis [33], where sets of exponential functions were used to derive the coefficients of the methods for first order ODEs. Methods using trigonometric polynomials have also been considered; for theoretical aspects see [34]. Salzer [35] assumed that the solution is a linear combination of trigonometric functions, of the form

$$y(x) = \sum_{j=0}^{J} [a_j \sin(jx) + b_j \cos(jx)], \tag{2.7}$$

with arbitrary constant coefficients a_j and b_j, to obtain predictor–corrector methods which are exact for this form; expressions of the coefficients of these methods are given in that paper for small values of J.

Versions for approximations which are exact for functions other than polynomials have been developed also for quadrature, see, e.g., [36], [37], [38], [39], [40], [41], [42], [43], and for interpolation, see [44]. Different techniques have been used but the exponential fitting has the advantage that it gives us the possibility of treating the things in an unitary way. As a matter of fact, for given M the exponential fitting allows using reference sets of the general form

$$y(x) = x^k \exp(\mu_i x),$$
$$k = 0, 1, 2, \ldots, m_i - 1, \; i = 1, 2, \ldots, I. \tag{2.8}$$

The values of I and of multiplicities m_i depend on M. We must have

$$M = m_1 + m_2 + \cdots + m_I \tag{2.9}$$

(this is called a selfconsistency condition) but there is a big flexibility otherwise; different assignments will lead to different coefficients. Thus, for the method of Numerov ($M = 6$) if $I = 1$, $\mu_1 = 0$ and $m_1 = 6$ we reobtain the classical algorithm but when $I = 3$, $\mu_1 = 0$, $\mu_2 = -\mu_3 = \mu$ where μ is either purely real or imaginary, and $m_1 = 4$, $m_2 = m_3 = 1$, we get the version of Raptis and Allison [19].

Although the set (2.8) is so general, forms which contain pairs of frequencies with opposite signs are preferred, viz.:

$$y(x) = 1, x, x^2, \ldots, x^K, \exp(\pm\mu_i x), x\exp(\pm\mu_i x), \ldots,$$
$$x^{P_i}\exp(\pm\mu_i x), \quad i = 1, 2, \ldots, I, \tag{2.10}$$

with the selfconsistency condition

$$M = 1 + K + 2I + 2(P_1 + P_2 + \cdots + P_I), \tag{2.11}$$

and the simplest case $I = 1$ of this,

$$y = 1, x, x^2, \ldots, x^K, \exp(\pm\mu x), x\exp(\pm\mu x), \ldots,$$
$$x^P \exp(\pm\mu x), \tag{2.12}$$

with the selfconsistency condition

$$M = 3 + K + 2P. \tag{2.13}$$

One of the reasons behind this preference is that it allows a direct treatment of oscillatory functions. If all frequencies are imaginary then these sets can be expressed in terms of trigonometric functions. Thus with $\mu = i\omega$ the set (2.12) becomes

$$y = 1, x, x^2, \ldots, x^K, \qquad \{x^m \sin(\omega x), x^m \cos(\omega x)\},$$
$$m = 0, 1, 2, \ldots, P, \tag{2.14}$$

and then the exponential fitting becomes a trigonometric fitting.

For clarity we will distinguish between approximations described by single formulas and those which need sets of formulas. The multistep algorithms for differential equations and the Newton–Cotes rule for quadrature are of the first type, to be contrasted by the Runge–Kutta algorithms with consist of sets of formulae, one for each internal stage and for the external stage. These subclasses will be treated separately.

3. Single formula approximations

Here we consider operations covered by one operator $\mathcal{L}$ whose general form is

$$\mathcal{L}[h, \boldsymbol{a}]y(x) = h^l \left[\frac{1}{h} \int_{x-h}^{x+h} g(x')y(x')\,dx' + \sum_{i=1}^{n}\sum_{k=0}^{m-1} h^k a_{ki} y^{(k)}(x + x_i h) \right]. \tag{3.1}$$

It contains the integral of $y(x)$ and the values of y and of a number of its derivatives at certain abscissa points in $[x-h, x+h]$; $\boldsymbol{a}$ collects all coefficients a_{ki}. The h^k factors were introduced to secure that the coefficients a_{ki} are dimensionless, while the front factor h^l and function g in the integrand were introduced in order to reproduce particular forms existing in the literature. $g(x)$ must be either a number (typically 0 or 1) or a delta function.

There is a vast variety of operations covered by such $\mathcal{L}$, and here are some simple illustrations:

Multistep algorithms for differential equations: Numerov rule (2.4) corresponds to $l = g = 0$, $n = m = 3$, $x_1 = -1$, $x_2 = 0$, $x_3 = 1$, and all $a_{ki} = 0$ except for $a_{01} = a_{03} = 1$, $a_{02} = a_0$, $a_{21} = a_{23} = -b_0$ and $a_{22} = -b_1$.

Quadrature rules: Simpson rule

$$\int_{X-h}^{X+h} y(x')dx' \approx h\,[a_1 y(X-h) + a_2 y(X) + a_3 y(X+h)], \tag{3.2}$$

(for the classical version the coefficients are $a_1 = a_3 = 1/3$, $a_2 = 4/3$) corresponds to $l = g = 1$, $n = 3$, $m = 1$, $x_1 = -1$, $x_2 = 0$, $x_3 = 1$, and all $a_{ki} = 0$ except for $a_{01} = -a_1$, $a_{02} = -a_2$, $a_{03} = -a_3$.

Interpolation: Interpolation of a function in terms of values of function and its first derivative at the endpoints of the interval:

$$y(X+th) \approx a_0(t)y(X-h) + a_1(t)y(X+h) + h[b_0(t)y'(X-h) + b_1(t)y'(X+h)], \quad -1 \le t \le 1 \tag{3.3}$$

has operator $\mathcal{L}$ of form (3.1) with $l = 1$, $g(x') = \delta(x' - th)$, $n = m = 2$, $x_1 = -1$, $x_2 = 1$, $a_{0i} = -a_i(t)$, $a_{1i} = -b_i(t)$.

3.1. Ixaru's six-step flow chart

This was first formulated in [25] and it is also explained in book [1]. Its purpose is to help deriving the coefficients of ef-based formulae with $\mathcal{L}$ of form (3.1) and evaluating the error in an efficient way for reference sets of the form (2.10).

The main ingredients are the moments and the reduced moments. The moments, classical L_m and ef-based E_m, are defined as follows:

$$L_m := \mathcal{L}[h, \boldsymbol{a}]x^m\,|_{x=0}, \qquad E_m := \mathcal{L}[h, \boldsymbol{a}]x^m \exp(\mu x)\,|_{x=0}, \tag{3.4}$$

for $m = 0, 1, 2, \ldots$. L_m depends on h and $\boldsymbol{a}$, while E_m on h, $z = \mu h$ and $\boldsymbol{a}$ but the dependence on h factorizes out:

$$L_m(h, \boldsymbol{a}) = h^{l+m} L_m^*(\boldsymbol{a}),$$
$$E_m(h, z, \boldsymbol{a}) = h^{l+m} E_m^*(z, \boldsymbol{a}). \tag{3.5}$$

L_m^* and E_m^* are called reduced moments. Two useful properties are: (i) Reduced moments with higher index result by successive differentiation of E_0^* with respect to z,

$$E_m^*(z, \boldsymbol{a}) = \frac{\partial^m E_0^*(z, \boldsymbol{a})}{\partial z^m}. \tag{3.6}$$

(ii) Classical and ef-based reduced moments are related,

$$L_m^*(\boldsymbol{a}) = \lim_{z\to 0} E_m^*(z, \boldsymbol{a}). \tag{3.7}$$

The six-step flow chart collects a number of theoretical results in ready-to-use form:

Step i. Choose the appropriate form of $\mathcal{L}[h, \boldsymbol{a}]$ (e.g., (2.4) for the Numerov method) and find the expressions of its classical reduced moments $L_m^*(\boldsymbol{a})$, $m = 0, 1, 2, \ldots$.
Hint: Write the expression of $E_0^*(z, \boldsymbol{a})$, then differentiate with respect to z and take the limit $z \to 0$.

Step ii. Examine the algebraic system

$$L_m^*(\boldsymbol{a}) = 0, \quad m = 0, 1, 2, \ldots, M-1 \tag{3.8}$$

to find out the maximal M for which this is compatible. For the Numerov method we have $L_0^*(\boldsymbol{a}) = 2 + a_1$, $L_2^*(\boldsymbol{a}) = 2(1 - 2b_0 - b_1)$, $L_{2k}^*(\boldsymbol{a}) = 2 - 4k(2k-1)b_0$, $k = 2, 3, \ldots$, $L_{2k+1}^*(\boldsymbol{a}) = 0$, $k = 0, 1, \ldots$, such that it easy to find out that $M = 6$.

Step iii. Using the expression of $E_0^*(z, \boldsymbol{a})$ write the expressions of

$$G^+(Z, \boldsymbol{a}) := \frac{1}{2}[E_0^*(z, \boldsymbol{a}) + E_0^*(-z, \boldsymbol{a})], \tag{3.9}$$

and

$$G^-(Z, \boldsymbol{a}) := \frac{1}{2z}[E_0^*(z, \boldsymbol{a}) - E_0^*(-z, \boldsymbol{a})], \tag{3.10}$$

where $Z := z^2$. Notice that the argument Z is real irrespective of whether μ is real or purely imaginary. Also write the expressions of their derivatives $G^{\pm(p)}(Z, \boldsymbol{a})$, $p = 1, 2, \ldots$ with respect to Z.
Hint: express $G^{\pm}(Z, \boldsymbol{a})$ in terms of the functions $\eta_s(Z)$, $s = -1, 0, 1, \ldots$ (see Appendix). One of the advantages will be a direct evaluation of the derivatives.

Step iv. Choose the reference set of M functions of form (2.10) which is appropriate for the given form of $y(x)$ and satisfies the selfconsistency condition (2.11).
Remark 1: The selfconsistency condition implies that M and K are of different parities: if M is even/odd then K is odd/even.
Remark 2: The reference set is characterized by the integer parameters I, K and P_i, $i = 1, \ldots, I$. The set in which there is no classical component is identified by $K = -1$ while the set in which there is no exponential fitting component with the pair of frequencies $\pm\mu_i$ has $P_i = -1$. Parameters P_i are called levels of tuning.
Remark 3: In most applications only one pair of frequencies, set (2.12), was considered. For $M = 6$ (as for the Numerov method) we have four possible variants: $K = 5, P = -1$ (classical version, abbreviated herein after S_0); $K = 3, P = 0$ (S_1); $K = 1, P = 1$ (S_2) and $K = -1, P = 2$ (S_3). The last is the best suited for functions of the form

$$y(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x) \quad \text{or} \quad y(x) = f_1(x)\sinh(\lambda x) + f_2(x)\cosh(\lambda x) \tag{3.11}$$

corresponding to imaginary $\mu = i\omega$ and real $\mu = \lambda$, respectively.
Remark 4: Accidental situations exist when the selfconsistency condition is violated. A situation of this type and a procedure adapted for the treatment of such a special case is presented in Chapter 4 of book [1].

Step v. Solve the algebraic system

$$L_k^*(\boldsymbol{a}) = 0, \quad 0 \le k \le K, \qquad G^{\pm(p)}(Z_i, \boldsymbol{a}) = 0, \quad 0 \le p \le P_i, i = 1, 2, \ldots, I, \tag{3.12}$$

for the coefficients $\boldsymbol{a}$ of the ef-based formula, where $Z_i := \mu_i^2 h^2$.

Step vi. Here we distinguish between the local truncation error, denoted *LTE*, and its leading term, denoted *lte*. If $\boldsymbol{a}(\boldsymbol{Z})$ are the obtained coefficients where $\boldsymbol{Z} = [Z_1, Z_2, \ldots, Z_I]$ then the leading term of the error is

$$lte_{ef} = (-1)^{P^*+I} h^{I+M}\, T(\boldsymbol{Z}) D^{K+1} O_1 O_2 \cdots O_I y(X), \tag{3.13}$$

where X is some point in the interval of interest, $P^* := P_1 + \cdots + P_I$, and

$$T(\boldsymbol{Z}) = \frac{L_{K+1}^*(\boldsymbol{a}(\boldsymbol{Z}))}{(K+1)! Z_1^{P_1+1}\cdots Z_I^{P_I+1}}, \qquad D^m := \frac{d^m}{dx^m}$$

$$O_i := (D^2 - \mu_i^2)^{P_i+1}.$$

As for the true local truncation error *LTE*, this is a sum of two terms of form (3.13). Specifically, as shown in [24] on the case of one single frequency (2.12), two functions $T^{\pm}(Z)$ ($T^+(Z) \ge 0, T^-(Z) \le 0$) with the property that $T^+(Z) + T^-(Z) = T(Z)$ and two points $\eta^{\pm} \in (x-h, x+h)$ exist, such that the error is

$$LTE_{ef} = (-1)^{P^*+I} h^{I+M}[T^+(Z)\, D^{K+1} O_1 O_2 \cdots O_I y(\eta^+) + T^-(Z)\, D^{K+1} O_1 O_2 \cdots O_I y(\eta^-)]. \tag{3.14}$$

This result is certainly important from a theoretical point of view, but not only, because the dependence on Z in $T^{\pm}$ may be quite different from that of their sum T. Think of an example of a case when $T^+(Z) = 1/Z + 1/Z^2$ and $T^-(Z) = -1/Z$. When $Z \to \infty$ their sum $T = 1/Z^2$ falls down faster than T^+ and therefore evaluations based on the *lte* may be inaccurate. Fortunately, such situations are rather rare in current practice. For an exceptional case see [24].

To illustrate the output of the six-point scheme we list below the coefficients of the three genuine ef versions of the Numerov method and their *lte*-s in terms of η functions. For details see [25,1]. For the form of the true LTE_{ef} see [45].

S_1, [19]: $a_1(Z) = -2$,

$$b_0(Z) = \frac{(\eta_0(Z/4)+1)(\eta_0^2(Z/16) - 2\eta_1(Z/4))}{8\eta_0^2(Z/4)}, \tag{3.15}$$

$$b_1(Z) = 1 - 2b_0(Z),$$

$$lte_{S_1} = -h^6 \frac{1 - 12b_0(Z)}{12Z}(-\mu^2 y^{(4)}(x_n) + y^{(6)}(x_n)). \tag{3.16}$$

S_2, [21]:

$$a_1(Z) = -2, \qquad b_0(Z) = \frac{\eta_1(Z/4)}{4\eta_{-1}(Z/4)}, \tag{3.17}$$

$$b_1(Z) = \eta_0^2(Z/4) - 2b_0(Z)\eta_{-1}(Z),$$

$$lte_{S_2} = h^6 \frac{Z^2\eta_0(Z) - 4(\eta_{-1}(Z)-1)^2}{Z^4\eta_0(Z)}[\mu^4 y''(x_n) - 2\mu^2 y^{(4)}(x_n) + y^{(6)}(x_n)]. \tag{3.18}$$

S_3, [22]:

$$a_1(Z) = -(6\eta_{-1}(Z)\eta_0(Z) - 2\eta_{-1}^2(Z) + 4)/D(Z),$$
$$b_0(Z) = \eta_1(Z)/D(Z), \tag{3.19}$$
$$b_1(Z) = (4\eta_0^2(Z) - 2\eta_1(Z)\eta_{-1}(Z))/D(Z),$$

where $D(Z) = 3\eta_0(Z) + \eta_{-1}(Z)$,

$$lte_{S_3} = -h^6 \frac{N(Z)}{F(Z)}[-\mu^6 y(x_n) + 3\mu^4 y^{(2)}(x_n) - 3\mu^2 y^{(4)}(x_n) + y^{(6)}(x_n)] \tag{3.20}$$

where $N(Z) = 6\eta_0(Z) + 2\eta_{-1}(Z) - 6\eta_{-1}(Z)\eta_0(Z) + 2\eta_{-1}^2(Z) - 4$ and $F(Z) = Z^3D(Z)$. Notice that a single formula is needed for each coefficient; no series expansion is required; compare b_0 in (3.15) and (2.7). Also notice that the coefficients are not defined for certain negative values of Z. Thus for S_1 the denominator of b_0 vanishes when $Z = -(2n\pi)^2$, $n = 1, 2, \ldots$. These are called *critical values*.

3.2. Multistep algorithms for differential equations

An r-th order equation of the form $y^{(r)} = f(x, y)$ has to be solved, and an s-step algorithm for its solution has the form

$$\sum_{j=0}^{s} a_j y_{n+j} = h^r \sum_{j=0}^{s} b_j f(x_{n+j}, y_{n+j}), \tag{3.21}$$

where $a_s = 1$ and $|a_0| + |b_0| \neq 0$. It allows computing the solution y_{n+s} at point x_{n+s} if all y_{n+j}, $j = 0, 1, \ldots, s-1$ are known. In most cases only equations of low order ($r = 1, 2$) are encountered. For classical algorithms the coefficients a_j and b_j are constants but for the ef-based versions they depend on the products $z_i = \mu_i h$, where μ_i are the frequencies involved.

Two specific issues are of direct interest: convergence of the algorithm, and how to choose the frequencies in order to obtain the maximal benefit in runs.

Convergence. For classical algorithms, a well known theorem from Dalquist says that the necessary and sufficient conditions for convergence are that the algorithm is consistent and zero-stable. This holds also true for ef-based algorithms but, because their coefficients are no longer constants the concepts of consistency and stability have to be adapted. Since all such things were explained at large in [1] they will not be repeated here. We only mention the main results:

Consistency is related to the value of M, Eq. (2.9) which is also the exponent of h in the expression of the *lte*, see Eq. (3.13) for that particular case. The algorithm is said to be of the order $p = M - r$ and it is consistent if $p \geq 1$.

The stability regards the way how the errors accumulate when the solution is propagated along the interval of interest. The zero-stability refers to the limit case $h \to 0$ but in applications where only significantly nonvanishing steps are used, of course. This is why the examination of the latter case is of major importance, and this forms the object of the linear stability theory. In [1] the first and second order equations were examined in detail in the ef context. The idea consists of choosing a differential equation whose analytic solution does not increase indefinitely when $x \to \infty$ and then checking whether the numerical solution conserves this property. For first and second order equations the test equation is $y' = \lambda y, x \geq 0$ with $Re\,\lambda < 0$, and $y'' = -k^2 y, x \geq 0$ with $k > 0$, respectively. Application of an s-step method on the test equation will lead to an s-order difference equation whose characteristic equation has s roots and the stability properties depend on the magnitude of these roots. For the versions presented above for the Numerov method with $\theta = \omega h$ and $Z = -\theta^2$ the second order difference equation is

$$y_{n+1} - 2R(\nu;\theta)y_n + y_{n-1} = 0, \quad n = 1, 2, \ldots \tag{3.22}$$

where $\nu = kh$. Function

$$R(\nu;\theta) = -\frac{a_1(-\theta^2) + \nu^2 b_1(-\theta^2)}{2[1 + \nu^2 b_0(-\theta^2)]} \tag{3.23}$$

is called stability function. Notice that ν depends on the test equation but θ on the numerical method, and also that there is no θ dependence in the classical version S_0. The characteristic equation is $d^2 - 2R(\nu;\theta)d + 1 = 0$ and if $R(\nu;\theta) < 1$ the two roots are $d_1 = \exp(i\rho h)$ and $d_2 = \exp(-i\rho h)$. If so, the difference equation has the general solution

$$\begin{aligned} y_n &= C_1 \exp(i\rho nh) + C_2 \exp(-i\rho nh) \\ &= (C_1 + C_2)\cos(\rho x_n) + i(C_1 - C_2)\sin(\rho x_n), \quad x_n = nh, \end{aligned}$$

where C_1, C_2 are arbitrary constants, and this is of the same form as the analytic solution. For contrast, if $R(\nu;\theta) > 1$, one of the roots is greater than zero in magnitude and therefore the numerical solution will increase indefinitely. In short the stability condition is $R(\nu;\theta) < 1$, and the regions in the ν, θ plane where this condition holds true are called stability regions.

These regions are presented on Fig. 1. We see that for all versions the origin belongs to the stability region and therefore they are convergent. We also see that the bisecting line $\theta = \nu$ belongs to the stability region for all ef-based versions. As for the extension of the stability region, this differs from one version to another, and, as a rule, it extends down when the tuning factor P is increased.

P-stability. This concept refers to second order equations of form (2.2) and it is described in detail in [23,1] for classical and genuine ef-based methods. To put it on an intuitive basis, let us refer to the versions of the Numerov method and the associate ν, θ plane. Each version, e.g. S_1, is actually a family of methods where each individual method is fixed by the value of ν. On that plane any such individual method in this family is represented by a horizontal line, and the method is said to be P-stable if the corresponding line is integrally placed inside the stability region. However, we see that this condition is never met in any of the four graphs, and therefore none of the methods discussed above is P-stable. This specification seems necessary because some authors including Wang [46] look along the bisecting line $\nu = \theta$ to conclude that the method is P-stable; the P-stability is also discussed in [47]. It is true that this line is inside the stability region for all ef-based versions but that line does not correspond to a fixed method. As a matter of fact, the P-stable two-step method in [23] has a low order, $p = 2$. In [48] P-stable methods methods of arbitrary high-order have been considered. It can be proved that the symplectic EF-Gauss method in [49,50] is also P-stable. In addition, [51] provides interesting examples of arbitrary high-order P-stable EF-methods. Conditionally P-stable methods also exist, see [52].

What influence may have the stability properties in current runs? Let us place ourselves in the situation when we need only qualitative information on the behavior of the solution. Thus we assume that the true frequency is $k = 16$ but that some separate estimations have wrongly indicated that $\omega = 20$ would be a good guess, and take $h = 0.5$. The point $(\nu = 8, \theta = 10)$ is inside the stability region for S_1 but not for S_2 and S_3. This means that there are real chances with S_1 for a qualitative description for the real solution (e.g., that it is oscillating) but not with the other two, in spite of the fact that these have a higher tuning parameter.

Choosing the frequencies. The formula of the *lte* has three factors: a power of h (which fixes the order p of the method; for a second order equation we have $p = M - 2$), a function which depends on the used frequencies (function T), and a factor which combines the frequencies with the solution and its derivatives. The natural way to find suited values of the frequencies consists of vanishing the differential factor and then computing the roots of the resulting equation. Thus, for version S_1 this vanishes when

$$\mu^2 = y^{(6)}(x_n)/y^{(4)}(x_n). \tag{3.24}$$

Approaches in this spirit are reported in the literature, e.g., [53–56], but technical problems appear when we want to put them into practice. For example, a reasonable accurate determination of the fourth and sixth order derivatives of the solution is needed for (3.24), and this is rather difficult for general $f(x, y)$. This is why

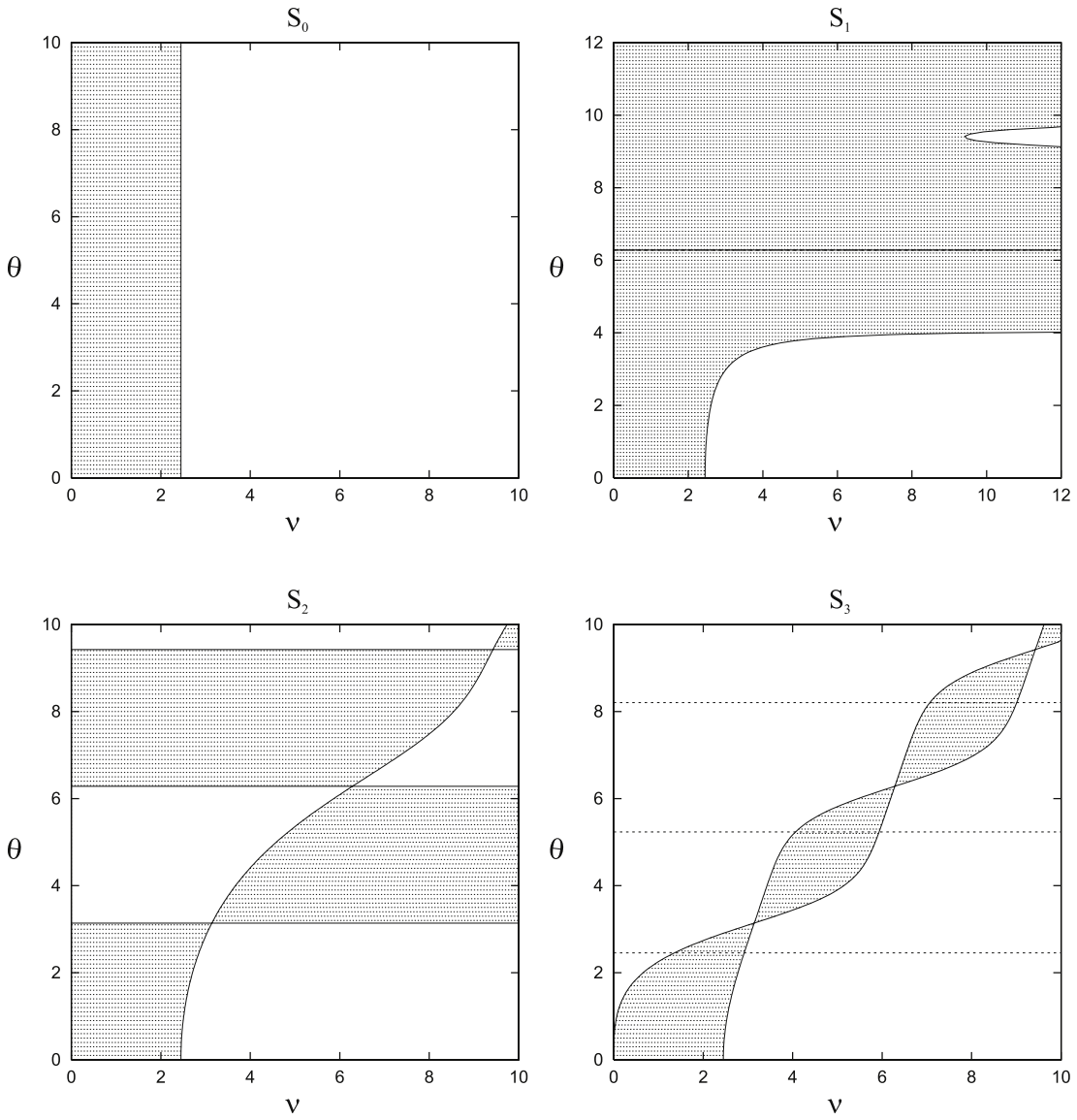

Fig. 1. The stability maps for versions S_0, S_1, S_2 and S_3 of the Numerov method.

equations where different ways are available became so popular. Such a case is when $f(x, y)$ is linear in y, with the Schrödinger equation

$$y'' = (V(x) - E)y, \quad x \in [a, b], \tag{3.25}$$

as its standard representative. If on a subinterval $[x_{\min}, x_{\max}]$ the potential function has a weak variation, then a constant approximation $\overline{V}$ is reasonable. The general solution of the equation with this $\overline{V}$ is a linear combination with constant coefficients of the form

$$y = \begin{cases} f_1 \sin(\omega x) + f_2 \cos(\omega x), & \omega = \sqrt{E - \overline{V}} \quad \text{if } E > \overline{V}, \\ f_1 \sinh(\lambda x) + f_2 \cosh(\lambda x), & \lambda = \sqrt{\overline{V} - E} \quad \text{if } E \le \overline{V}. \end{cases}$$

The point is that we can accept that the solution with the original $V(x)$ has the same form except that coefficients are now slowly varying functions of x, as in Eq. (3.11), see [21], and therefore the version S_3 with the fitting frequency $\mu = i\omega$ for $E > \overline{V}$ and $\mu = \lambda$ for $E \le \overline{V}$ is the best suited of all Numerov versions on the mesh points x_n in the quoted subinterval.

We now present a numerical example intended to illustrate how versions of the Numerov method with increasing values of the tuning parameter P help improve the accuracy of the numerical solution. Theory shows that when E increases then the error of versions S_0 to S_3 increases as $E^3, E^2, E^{3/2}$ and E, respectively, see [21]; a recent separate investigation is in [57]. We take the Woods–Saxon potential

$$V(x) = v_0/(1 + t) + v_1 t/(1 + t)^2, \quad t = \exp[(x - x_0)/a], \tag{3.26}$$

where $v_0 = -50$, $x_0 = 7$, $a = 0.6$ and $v_1 = -v_0/a$. Its shape is such that only two values for $\overline{V}$ are sufficient:

$$\overline{V} = \begin{cases} -50 & \text{if } 0 \le x \le 6.5 \\ 0 & \text{if } x > 6.5 \end{cases}$$

such that the parameters are updated only twice for each E. We solve the resonance problem which consists of the determination of the positive eigenvalues corresponding to the boundary conditions

$$y(0) = 0, \qquad y(x) = \cos(E^{1/2}x) \quad \text{for some big } x.$$

The physical interval $x \ge 0$ is cut at $b = 20$, and the eigenvalues are obtained by shooting at $x_c = 6.5$. For any trial value for E the solution is propagated forwards with the starting values $y(0) = 0, y(h) = h$ up to $x_c + h$, and backwards with the starting values $y(b) = \cos(E^{1/2}b), y(b - h) = \cos(E^{1/2}(b - h))$ up to x_c. If E is an eigenvalue, the forwards and backwards solutions are proportional

Table 1
Absolute errors $E_{exact} - E_{comput}$ in 10^{-6} units from the four versions of the Numerov method for the resonance eigenenergy problem of the Schrödinger equation in the Woods–Saxon potential (3.26) and its piecewise constant approximation $\overline{V}$. The empty areas indicate that the corresponding errors are bigger than the format adopted in the table.

h	S_0	S_1	S_2	S_3
$E_{exact} = 53.588852$				
1/16	−259 175	6 178	−1 472	587
1/32	−15 872	367	−84	35
1/64	−989	22	−5	1
1/128	−62	1	0	0
$E_{exact} = 163.215298$				
1/16		79 579	−9 093	721
1/32	−595 230	4 734	−525	46
1/64	−36 661	292	−32	2
1/128	−2 287	18	−1	0
$E_{exact} = 341.495796$				
1/16		661 454	−40 122	1 600
1/32		36 703	−2 116	126
1/64	−560 909	2 215	−126	7
1/128	−34 813	136	−8	0

and then the numerical values of the products $y^f(x_c+h)y^b(x_c)$ and $y^b(x_c+h)y^f(x_c)$ must coincide. That is to say that the resonance eigenenergies are searched for by vanishing the mismatch function

$$\Delta(E) = y^f(x_c+h)y^b(x_c) - y^b(x_c+h)y^f(x_c).$$

The error in the eigenvalues will then reflect directly the quality of the solvers for the initial value problem used for the determination of the solution $y(x)$.

In Table 1 we list the absolute errors in three such eigenvalues for all four versions of the Numerov method; the reference values, which are exact in the written figures, have been generated in a separate run with the method CPM(2) from [14] at $h = 1/16$. It is seen that, as expected, all these versions are of order four but the way in which the error increases with the energy differs from one version to another, much like the theoretical prediction.

Many other ef-based multistep methods have been investigated in the literature but the terminology used in some of these papers differs from that presented above. Thus, in a series of papers, e.g., [58], Simos introduces methods with vanished phase-lag and its derivatives. The analogy is direct: a method with vanished phase-lag relative to frequency ω and k derivatives of this is a method corresponding to set (2.10) for $\mu_1 = i\omega$ and $P_1 = k$ or, if only one frequency is present, to set (2.12) with $\mu = i\omega$ and $P = k$. This allows indexing these methods by the parameters M, I, K, P_i from the six-point scheme, and in this way the comparisons become easier. Thus the methods developed in [59] are versions of a four-step method where some coefficients are fixed from the very beginning, and the others are determined by asking that the phase-lag is vanishing. All versions have $M = 6, I = 1$ and $(K, P) = (3, 0)$ and therefore their accuracy is close to that of S_1.

The methods presented in [60] are 10-step methods with $M = 14$ (that is, of order 12) and $I = 1$ in two versions, with $(K, P) = (11, 0)$ and $(13, 1)$, respectively.

In [61] six versions of a 14-step method are presented. They correspond to $M = 16$, $I = 1$ and $(K, P) = (13, 0), (11, 1), (9, 2), (7, 3), (5, 4), (3, 5), (1, 6)$. Note in passing that the optimal version for the Schrödinger equation would be $(-1, 7)$, but this is not investigated.

The Cowell method is considered in [62] and a separate procedure for the computation of the coefficients is developed when a few pairs of frequencies are involved, as in set (2.10). However, these authors treat in detail only the case of a single pair $I = 1$ and they give the coefficients for $M = 6$, $(K, P) = (3, 0), (1, 1)$; $M = 8$, $(K, P) = (5, 0), (3, 1), (1, 2)$; $M = 10$, $(K, P) = (7, 0), (5, 1), (3, 2)$ with imaginary μ.

Quite special is one of the versions reported by Simos, [58]. On starting from a version proposed by Wang [46] with $M = 8, I = 1$, $(K, P) = (5, 0)$, two extensions with the same M are developed. The first has $I = 2$ and what is unusual is that the two frequencies are imaginary and real, respectively: $\mu_1 = i\omega$ and $\mu_2 = \sqrt{3}\omega$. This version has $(K = -1, P_1 = 2, P_2 = 0)$. The second version has $I = 1$, imaginary μ and $(K, P) = (-1, 3)$ such that it is maximally fitted for the Schrödinger equation.

All these results allow drawing some conclusions. First, as expected, M increases with the number of steps and, also as expected, the expressions of the coefficients become more and more complicated. Possible solutions would consist in either making coefficient generating codes available or converting these expressions in terms of η functions. A conversion code in Mathematica is available [63]. Second, the extension of the stability regions is more and more reduced when M and/or P are increased, and therefore the computation is increasingly affected by stability restrictions.

3.3. Other ef-based numerical operations

The problems arising for such operations are comparatively simpler than for the methods for differential equations because the values of the involved frequencies are usually known in advance at least approximately, and therefore there is no need for any extra effort to evaluate them, and also because difficult problems like stability do not appear.

Numerical differentiation. EF-based versions of standard formulae like three or five-point formulae for the first derivative or three-point formula for the second derivative are available, [25,1]. Ad-hoc formulae have also been produced, as, for example, a three-point formula for the first derivative which uses not only the values of the function at the mesh points but also of its second derivative, [1]. This is a direction to be considered attentively in the future because in typical runs such values happen to be available from the previous steps of the computation process, and thus the use of such information helps increasing the accuracy at no extra cost.

Quadrature. For the ef-based version of the Simpson quadrature rule at various levels of tuning, see [25] and references therein. As for the ef-based version of the Newton–Cotes rule in standard and extended form (that is, where not only the values of the integrand but also those of a number of its derivatives are known) see [64–66]. The Gauss–Legendre quadrature rule appropriate for oscillatory integrands has also been investigated, [67–70]. As a matter of fact, an investigation on the Gauss–Laguerre rule may be of acute interest for applications.

Also related is the approach of the Volterra integral equations in [71].

Interpolation. Frequency-dependent interpolation rules and their error analysis were considered in [72,73].

4. Multiple formulae approximations: the case of multistage methods for ordinary differential equations

The need for multiple formulae is generally related to the multistage nature of the underlying methods. Examples include the Runge–Kutta methods for first order ODEs, Runge–Kutta-Nyström methods, two-step Runge–Kutta methods and two-step hybrid methods for second order ODEs. Modern improvements to some of these algorithms are also recalled, in particular RK methods with equation depending coefficients [74,75].

4.1. Runge–Kutta methods

The algorithm of the s-stage RK method for the first order ODE of form $y' = f(x, y)$ is

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, 2, \ldots, s, \tag{4.1}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_j h, Y_i) \tag{4.2}$$

see, e.g. [76]. The stage abscissa points $x_n + c_j h$ are generally taken in $[x_n, x_{n+1} = x_n + h]$. The following $s + 1$ linear operators are associated

$$\mathcal{L}_i[h, \boldsymbol{a}]y(x) = y(x + c_i h) - y(x) - h\sum_{i=1}^{s} a_{ij} y'(x + c_j h), \quad i = 1, 2, \ldots, s, \tag{4.3}$$

$$\mathcal{L}[h, \boldsymbol{b}]y(x) = y(x + h) - y(x) - h\sum_{i=1}^{s} b_i y'(x + c_j h) \tag{4.4}$$

which provide the starting ingredient to build up the ef version. For shortage in the notation, $\boldsymbol{a}$ is an s by s matrix which collects a_{ij}, $\boldsymbol{b} = \{b_1, b_2, \ldots, b_s\}$, and $\boldsymbol{c} = \{c_1, c_2, \ldots, c_s\}^T$ is a column vector.

The first attempt in this area is from Simos [77] for the four stage diagonally explicit method, that is with $s = 4$ and where only the diagonal elements of $\boldsymbol{a}$ are nonvanishing. Simos' method was re-examined by Vanden Berghe et al. (see [78,1]) who found out that this method is exact if $y(x) = 1, x$ or if the right hand term in the equation is simply $f(x, y) = \mu y$. They realized that, in order to obtain ef-based explicit RK methods corresponding to a wider functional set, more degrees of freedom have to be introduced in the algorithm. Specifically, they assumed a form containing extra multiplying factors γ_i of y_n in the internal stages formulae, viz.:

$$Y_i = \gamma_i y_n + h\sum_{j=1}^{s} a_{ij} f(x_n + c_j h Y_j), \quad i = 1, 2, \ldots, s \tag{4.5}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_j h Y_i). \tag{4.6}$$

They derived an ef-based explicit RK method which is exact if $y(x) = \exp(\pm\mu x)$, $\mu \in \mathbb{C}$ or if $f = 1$ or $f = x$, see also [79]. For $\mu = i\omega$, $\omega \in \mathbb{R}$ their method has the Butcher-like tableau

$$\begin{array}{c|c|c} \boldsymbol{c} & \boldsymbol{\gamma} & \boldsymbol{a} \\ \hline & & \boldsymbol{b} \end{array} \tag{4.7}$$

of the form

$$\begin{array}{c|c|ccc|c} 0 & 1 & & & & \\ 1/2 & \cos(\nu/2) & \dfrac{\sin(\nu/2)}{\nu} & & & \\ 1/2 & \dfrac{1}{\cos(\nu/2)} & 0 & \dfrac{\tan(\nu/2)}{\nu} & & \\ 1 & 1 & 0 & 0 & \dfrac{2\sin(\nu/2)}{\nu} & \\ \hline & & b_1 & b_2 & b_3 & b_4 \end{array} \tag{4.8}$$

with $\nu = \omega h$ and

$$b_1 = b_4 = \frac{2\sin(\nu/2) - \nu}{2\nu(\cos(\nu/2) - 1)},$$

$$b_2 = b_3 = \frac{\nu\cos(\nu/2) - 2\sin(\nu/2)}{2\nu(\cos(\nu/2) - 1)}.$$

In that paper the frequency ω has always been assumed as known in advance but in practice this has to be determined. This problem was examined in [80,1] and the used technique is similar with that around Eq. (3.24). The expression of the local truncation error of the method (4.8) is (see [80,1]):

$$LTE = -\frac{h^5}{2880}[(y^{(2)} + \omega^2 y)^{(3)} + \alpha\cdot(y^{(2)} + \omega^2 y)'' + \beta\cdot(y^{(2)} + \omega^2 y)' + \gamma\cdot(y^{(2)} + \omega^2 y)] + O(h^6)$$

where α, β and γ are functions depending on f and y. On this basis the value

$$\omega = \sqrt{-\frac{y^{(2)}(x_n)}{y(x_n)}}$$

is the recommended for the scalar equation. For a d-dimensional differential system, they suggest the estimation

$$\omega = \sqrt{-\frac{\sum_{t=1}^{d} y_t(x_n) y_t^{(2)}(x_n)}{\sum_{t=1}^{d} y_t(x_n)^2}}.$$

The expression of the occurring second derivatives can be directly computed from the differential system or numerically approximated by suited differentiation formulae involving the computed approximations to the solution. In the same paper [80] the authors derive an ef-based three-stage implicit RK method which is of order four and merges into the classical Lobatto IIIA method when $\nu \to 0$. In the context of Runge–Kutta–Nyström methods it is worth mentioning [81–83].

Recent contributions in the development of a theory of ef-based families of multistage methods which generalize RK formulae are the object of [84–96].

4.2. Error control

Up to now we have considered ef-based methods on a uniform grid but the practical efficiency is certainly increased by using a variable stepsize implementation. This asks for an estimate for the local error. The first problem for ef-based methods is the determination of the suitable frequency but once this frequency has been fixed some popular techniques for estimating the local error are at our disposal for being adapted for ef-based algorithms, see [1,78,79,97].

There are two main possible techniques. The first is based on the Richardson extrapolation (see, for instance, [98]). We apply the ef-based RK method of order p to compute the approximation y_{n+1} of the solution at x_{n+1}. The local error then is

$$y(x_{n+1}) - y_{n+1} = C(y, f)h^{p+1} + O(h^{p+2}),$$

where $C(y, f)$ is some weight function. We next compute a second, finer approximation by applying the same method twice with steplength $h/2$. Denoting this as z_{n+1}, the local error is now

$$y(x_{n+1}) - z_{n+1} = 2C(y, f)(h/2)^{p+1} + O(h^{p+2}).$$

The ready-to use expression of the error in the first calculation results directly:

$$y(x_{n+1}) - y_{n+1} \approx \frac{2^p(z_{n+1} - y_{n+1})}{2^p - 1}.$$

Notice that this method is rather time consuming: it requires the application of the algorithm three times on each step.

The second technique is faster. It consists of using an embedded pair of methods of different orders and taking the solution from the method with the highest order for reference. The first embedded pair of ef-based Runge–Kutta methods has been derived by Franco in [79] (also compare [1]). It consists of a pair of methods of orders 4 and 5 respectively, each of them being exact for $y(x) = \exp\{(\pm\mu x), \mu \in \mathbb{C}\}$, whose Butcher-like array

$\boldsymbol{c}$	$\boldsymbol{\gamma}$	$\boldsymbol{a}$
		$\boldsymbol{b}$
		$\bar{\boldsymbol{b}}$

has the form

0	1					
$\frac{1}{2}$	$\eta_{-1}(Z/4)$	$\eta_0(Z/4)/2$				
$\frac{1}{2}$	$\frac{1}{\eta_{-1}(Z/4)}$	0	$\frac{\eta_0(Z/4)}{2\eta_{-1}(Z/4)}$			
1	1	0	0	$\eta_0(Z/4)$	0	
$\frac{3}{4}$	1	$\frac{5}{32}$	$\frac{7}{32}$	a_{53}	a_{54}	0
		b_1	b_2	b_3	b_4	0
		$\bar{b}_1$	$\bar{b}_2$	$\bar{b}_3$	$\bar{b}_4$	$-\frac{16}{5}$

with

$$a_{53} = -\frac{32\eta_{-1}(Z/16) - 32\eta_{-1}(Z) + 3.5\eta_0(Z/4) + 5Z\eta_0(Z)}{16Z\eta_0(Z/4)},$$

$$a_{54} = \frac{5 - 64\eta_{-1}(Z/4)/(Z\eta_0(Z/4)) + 64/(Z\eta_0(Z/16))}{32},$$

$$b_1 = b_4 = \frac{\eta_0(Z/4) - 1}{2(\eta_{-1}(Z/4) - 1)},$$

$$b_2 = b_3 = \frac{\eta_{-1}(Z/4) - \eta_0(Z/4)}{2(\eta_{-1}(Z/4) - 1)},$$

$$\bar{b}_1 = \frac{3 - 3\eta_{-1}(Z) - 8Z\eta_0(Z/16) + 9.5Z\eta_0(Z/4)}{3Z\eta_0(Z/4) - 3Z\eta_0(Z)},$$

$$\bar{b}_2 = \bar{b}_3 = \frac{-16\eta_{-1}(Z/16) + 19\eta_{-1}(Z/4) - 3\eta_0(Z/4)}{3/4Z\eta_0^2(Z/16)},$$

$$\bar{b}_4 = \frac{3 - 3\eta_{-1}(Z) + 4Z\eta_0(Z/16) + 9.5Z\eta_0(Z/4) - 12Z\eta_0(9Z/16)}{3Z\eta_0(Z/4) - 3Z\eta_0(Z)}.$$

where $Z = (\mu h)^2$. It is tacitly assumed here that μ is either real or purely imaginary, such that Z is real. The gain in efficiency comes from the fact that the first four internal stages are identical in the two methods such that they should be computed once. Only the fifth internal stage in the second method and the external stages in the two have to be computed separately. We also mention that the above formulation of the coefficients in terms of the η functions has been derived in Ixaru's book [1], while Franco considered only the case of real μ to express them in terms of hyperbolic functions. Finally we remark that, for Z tending to 0, the embedded pair derived by Franco tends to the Zonnevald 4(3) pair [99], thus it can be seen as the exponential fitting adaptation of the latter. The ef adaptation of other embedded pairs is the object of [100], while the derivation of ef-based embedded pairs of Runge–Kutta–Nyström methods is reported in [101].

4.3. Collocation-based methods

Collocation methods are based on the idea of approximating the exact solution of a given differential equation by a suitable approximant, the *collocation function*, belonging to a chosen finite dimensional space and then imposing the condition that this function exactly satisfies the equation on a set of discrete points on the integration interval, called *collocation points*. The classical form of a collocation function is a polynomial but linear combinations of other functions, for example $1, x, x^2, \ldots, x^K, \exp(\pm\mu x)$, are also permitted. The ef-based collocation methods cover the latter case.

The problem of RK methods of collocation type enjoyed a sustained interest in the literature. Thus, for the classical case it is well known (see, for instance, [98,99]) that implicit Runge–Kutta methods based on Gauss–Legendre, Radau IIA and Lobatto IIIA nodes are of collocation type, thus the entries of the $\boldsymbol{a}$ matrix and the vector $\boldsymbol{b}$ of the weights are the values of the integrals

$$a_{ij} = \int_0^{c_i} L_j(t)dt, \qquad b_j = \int_0^1 L_j(t)dt, \quad i, j = 1, 2, \ldots, s,$$

where $L_j(t)$ is the j-th fundamental Lagrange polynomial. The corresponding exponential fitting version is the object of the paper [102], where the authors have focused their attention on methods using the Gauss–Legendre, Radau and Lobatto nodes, and studied their convergence and stability properties. For instance, by choosing the fitting space $\{1, x, \exp(\mu x)\}$, the exponentially fitted Lobatto IIIA method with two stages corresponds to the following (c, A, b^T)-Butcher tableau

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \dfrac{1 + e^{\nu}(\nu - 1)}{\nu(e^{\nu} - 1)} & 1 - a_{21} \\ \hline & a_{21} & a_{22} \end{array} \tag{4.9}$$

where $\nu = \mu h$. We observe that, differently from [78], the methods derived in [102] do not depend on the extra weight γ_i. The above method is convergent, since the local truncation error is

$$LTE = \frac{\mu y^{(2)} - y^{(3)}}{12} h^3 + O(h^4).$$

Concerning the stability properties, it is possible to prove that this method inherits the same stability properties of its classic analog, thus it is A-stable. A similar analysis for the methods using Gauss–Legendre and Radau IIA nodes is reported in [102].

The problem of choosing the collocation points in ef-based RK methods of collocation type has been discussed in [103]. These authors compared the cases of fixed and frequency-dependent collocation points and have shown that using fixed points is much more practical, especially for systems of differential equations.

Other contributions connected to this area are [104,82,105,44,106,83,107–109] and references therein.

4.4. Symplectic integrators

The numerical solution of Hamiltonian problems received special attention in the last decades, see [110] and the references therein. The central problem is here that numerical methods must be introduced which are able to preserve the invariants possessed by the continuous problem. This is typically achieved by symplectic Runge–Kutta methods, i.e. RK methods satisfying the additional algebraic constraint

$$\mathrm{diag}(\boldsymbol{b})\boldsymbol{a} + \boldsymbol{a}^T\mathrm{diag}(\boldsymbol{b}) - \boldsymbol{b}\boldsymbol{b}^T = 0,$$

because these numerically preserve quadratic invariants.

Since Hamiltonian problems frequently model phenomena in celestial mechanics, molecular dynamics, plasma physics and so on, which notoriously possess periodic or oscillatory functions, it becomes important to combine the advantages of symplecticness and special purpose methods (see [111–113]). A paper in this direction is due to Tocino and Vigo-Aguiar, who derived in [112] the conditions for a Runge–Kutta–Nyström method being symplectic. The authors focused their attention on the problem

$$y''(t) + \omega^2 y(t) = f(y(t)),$$

where $f(y)$ is the gradient of a potential scalar, and considered the family of Runge–Kutta–Nyström (RKN) methods for the above

problem, i.e.

$$y_{n+1} = Cy_n + hDy'_n + h^2 \sum_{i=1}^{s} \beta_i f(Q_i),$$
$$y'_{n+1} = Ay'_n + \frac{B}{h} y_n + h^2 \sum_{i=1}^{s} b_i f(Q_i), \tag{4.10}$$

where $Q_i = Cy_n + hD_i y'_n + h^2 \sum_{j=1}^{s} a_{ij} f(Q_j)$, $i = 1, 2, \ldots, s$. The following results holds.

Theorem 4.1. *The modified RKN scheme (4.10) is symplectic if and only if its parameters satisfy*

$$AC - BD = 1,$$
$$\beta_i \left(A - B\frac{D_i}{C_i} \right) = b_i \left(D - C\frac{D_i}{C_i} \right), \quad i = 1, \ldots, s,$$
$$b_i \left(\beta_j - a_{ij}\frac{C}{C_i} \right) + \beta_i a_{ij} \frac{B}{C_i} = b_j \left(\beta_i - a_{ji}\frac{C}{C_j} \right) + \beta_j a_{ji} \frac{B}{C_j}, \quad i < j = 1, \ldots, s.$$

No examples of methods have been derived in [112]. A more constructive approach for the derivation of symplectic methods for the problem

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}, \qquad \dot{q}_k = \frac{\partial H}{\partial p_k}, \quad k = 1, \ldots, d,$$

has been provided in [114] in the context of explicit RKN methods of the form

$$Y_i = y_n + c_i \gamma_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j h, Y_j), \quad i = 1, \ldots, s$$
$$y_{n+1} = g_1 y_n + h g_2 y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i f(t_n + c_i h, Y_i),$$
$$y'_{n+1} = g_3 y'_n + h \sum_{i=1}^{s} b_i f(t_n + c_i h, Y_i).$$

In the case $s = 2$, symplecticity is achieved if

$$g_1 g_3 = 1,$$
$$g_3 \bar{b}_1 - g_2 b_1 = 0,$$
$$g_3 + \bar{b}_2 + (g_1 c_2 \gamma_2 - g_2) b_2 = 0,$$
$$b_1 \bar{b}_2 - \bar{b}_1 b_2 + g_1 b_2 a_{21} = 0.$$

In correspondence to the abscissa vector $\boldsymbol{c} = \{0, 1\}^T$, the above system of equations is satisfied by the method whose Butcher array

$\boldsymbol{c}$	$\boldsymbol{\gamma}$	$\boldsymbol{a}$
		$\boldsymbol{b}^T$
		$\bar{\boldsymbol{b}}^T$

has the form

0	1	
1	$\frac{\sinh(\nu)}{\nu}$	$\frac{\cosh(\nu)-1}{\nu^2}$
		$\frac{\sinh(\nu)}{\nu(\cosh(\nu)+1)}$ $\quad b_1$
		a_{21} $\quad 0$

with $\nu = \mu h$, $g_1 = 1$, $g_2 = \gamma_2$ and $g_3 = 1$. The derived method is symplectic and exponentially fitted with respect to the fitting space $\{1, x, \exp(\mu x)\}$.

A famous symplectic RK method is that based on the Gauss–Legendre nodes. The ef adaptation of this method is due to Van de Vyver [50] and corresponds to the Butcher array (4.7)

$\frac{3-\sqrt{3}}{6}$	$\frac{2e^{\nu/2}(1+E+E^2+E^3)}{\sqrt{E}(1+E)^2(e^\nu+1)}$	$\frac{(e^\nu-1)(1+E^2)}{\nu(e^\nu+1)(1+E)^2}$	$\frac{2(e^\nu-E^2)}{\nu(e^\nu+1)(1+E)^2}$
$1-c_1$	γ_1	$\frac{2(e^\nu E^2-1)}{\nu(e^\nu+1)(1+E)^2}$	a_{11}
		$\frac{e^\nu-1}{\nu e^{c_1\nu}(1+E)}$	b_1

with $E = e^{\nu\sqrt{3}/3}$. Other symplectic (and also symmetric) ef-based RK methods have been presented in [115,116,49,117,118].

An interesting theoretical analysis of the canonical properties of ef-based RK methods is due to Calvo et al. [119], where the structure preservation properties are derived in terms of simple algebraic constraints which have to be fulfilled by the coefficients of the method. In particular, for ef-based RK method, the following results hold.

Theorem 4.2. *An EFRK method (4.5),*

(i) *preserves linear invariants;*
(ii) *preserves quadratic invariants if and only if* $\Omega_{ij} = b_j \gamma_j^{-1} a_{ji} + b_i \gamma_i^{-1} a_{ij} - b_i b_j = 0$, $1 \le i, j \le s$;
(iii) *is symplectic if* $\Omega_{ij} = 0$, $1 \le i, j \le s$.

4.5. A new perspective: Runge–Kutta methods with equation depending coefficients

The act of associating the $s + 1$ operators (4.3)–(4.4) to the algorithm (4.1)–(4.2) is a general practice in the literature of ef-based RK methods (see, e.g., [120,1,77,80,48]) but this was critically reconsidered in two recent papers, [74,75]. The point is that in spite of the error in computing y_{n+1} by (4.2) *cumulates* the error related to the final stage *and* those generated during the computation of the intermediary values Y_i in the internal stages, in Eqs. (4.3)–(4.4) each stage is treated *separately* and then the error contamination process is disregarded. Also, what we are actually interested in is the error in final output y_{n+1} not in the values of Y_i. This raises the problem of modifying the way of constructing the coefficients of the method such that the propagation of the error along the stages becomes visible.

In paper [74] the case of the explicit two-stage RK method

0		
c_2	a_{21}	
	b_1	b_2

is examined for the fitting space $\{1, \exp(\mu x), x\exp(\mu x)\}$.

Internal stages. In force of the localizing assumption $y_n = y(x_n)$ there is no error in Y_1 and therefore associating the operator

$$\mathcal{L}_2[h, \mathbf{a}]y(x)|_{x=x_n} = y(x_n + c_2 h) - y(x_n) - h a_{21} y'(x_n) \tag{4.11}$$

to the second internal stage $Y_2 = y_n + a_{21} f(x_n, Y_1)$ is just natural. By asking whether this is identically vanishing for $y(x) = 1$ and $\exp(\mu x)$ one obtains $a_{21}(z) = (\exp(c_2 z) - 1)/z$ and

$$lte = h^2 F(z)(y''(x_n) - \mu y'(x_n)),$$

where $F(z) = [-1 - c_2 z + \exp(c_2 z)]/z^2$. The error in Y_2 then is

$$LTE := y(x_n + c_2 h) - Y_2 = lte + \mathcal{O}(h^3). \tag{4.12}$$

External stage. The natural form of the operator to be associated to $y_{n+1} = h[b_1 f(x_n, Y_1) + b_2 f(x_n + c_2 h, Y_2)]$ is

$$\hat{\mathcal{L}}[h, \mathbf{b}]y(x)\big|_{x=x_n} = y(x_n + h) - y(x_n) - h(b_1 y'(x_n) + b_2 f(x_n + c_2 h, Y_2)), \tag{4.13}$$

but this cannot be treated in the usual way because it is nonlinear. However, since

$$\begin{aligned} y'(x_n + c_2h) &= f(x_n + c_2h, y(x_n + c_2h)) \\ &= f(x_n + c_2h, Y_2 + LTE) \\ &= f(x_n + c_2h, Y_2) + lte\, f_y(x_n + c_2h, Y_2) \\ &\quad + \mathcal{O}(h^3), \end{aligned} \tag{4.14}$$

and by neglecting the residual error $\mathcal{O}(h^3)$, one gets a linearized form of (4.13),

$$\begin{aligned} \mathcal{L}^R[h, \mathbf{b}]y(x)\big|_{x=x_n} &= y(x_n + h) - y(x_n) - hb_1y'(x_n) \\ &\quad - hb_2[y'(x_n + c_2h) \\ &\quad - hM_2F(z)(y''(x_n) - \mu y'(x_n))], \end{aligned} \tag{4.15}$$

with notation $M_2 = hf_y(x_n + c_2h, Y_2)$. The difference of this revised form (R) with respect to the standard (S) form (4.4) consists of the appearance of the last term which takes into account the error contamination effect. Asking whether each of the two forms is exact for $y(x) = 1, \exp(\mu x), x\exp(\mu x)$, it is obtained that

$$\begin{aligned} b_1^S(z) &= \frac{-1 - c_2z + \exp(z)(1 + (-1 + c_2)z)}{c_2z^2}, \\ b_2^S(z) &= \frac{1 - \exp(z) + z\exp(z)}{c_2z^2\exp(c_2z)}, \end{aligned} \tag{4.16}$$

$$b_1^R(z) = \frac{\alpha(z)M_2 + b_1^S(z)}{\gamma(z)M_2 + 1}, \qquad b_2^R(z) = \frac{b_2^S(z)}{\gamma(z)M_2 + 1},$$

$$\text{where } \gamma(z) = \frac{1 - \exp(c_2z) + c_2z}{c_2z^2\exp(c_2z)}, \tag{4.17}$$

$$\alpha(z) = \frac{(\exp(z) - 1)\gamma(z)}{z}.$$

For the new version we have

$$\begin{aligned} LTE^R &= -\frac{h^3}{12}(-2 + 3c_2)[y'''(x_n) - 2\mu y''(x_n) + \mu^2 y'(x_n)] \\ &\quad + O(h^4), \end{aligned} \tag{4.18}$$

and therefore it is generally of order 2. However, if $c_2 = 2/3$ then the order becomes 3.

Also instructing is another remark. The leading term of the LTE^R obviously vanishes for all three functions in the fitting space but this does not mean that the algorithm is exact for these and their linear combination. The reason is that when building up the operator (4.15) for the final stage the residual error $\mathcal{O}(h^3)$ of (4.12) was completely disregarded. The influence of this error, which vanishes only for $y(x) = 1, \exp(\mu x)$, is obviously like $\mathcal{O}(h^4)$ due to the factor h in (4.13). The consequence is that, in spite of the *lte* of Eq. (4.18) vanishing for all three functions, the algorithm is actually exact only for 1 and $\exp(\mu x)$ and their linear combination. A conclusion of the same type holds true for all ef-based RK algorithms.

In [75] Ixaru treats the three-stage explicit RK method

0			
c_2	a_{11}		
c_3	0	a_{23}	
	b_1	b_2	b_3

in the same way. He is interested to see in what extent such a treatment may produce different results than the standard treatment in the field, e.g. as in [98]. He takes the power function set for reference and obtains $a_{21} = c_2, a_{23} = c_3, b_i = b_i^{num}/b_i^{den}$ where

$$\begin{aligned} b_1^{num} &= c_3(3c_3 - 2) + c_2^2(6c_3 - 3) + c_2(2 - 6c_3^2) \\ &\quad + c_2^2(c_2 - 2c_2c_3 + 3c_3^2 - 1)M_2 \\ &\quad + (c_3 - 1)\{c_3[-3c_2^2 - c_3 + 2c_2(1 + c_3)]M_3 \\ &\quad + c_2^2c_3(c_2 - c_3 - 1)M_2M_3\}, \\ b_2^{num} &= 2 - 3c_3 + [2c_2 - 3c_2^2 + (c_3 - 1)c_3]M_3 \\ &\quad + (c_2 - 1)c_2^2M_2M_3, \\ b_3^{num} &= -2 + 3c_2 - (c_2 - 1)c_2M_2, \\ b_1^{den} &= c_2c_3B, \qquad b_2^{den} = c_2B, \qquad b_3^{den} = c_3B, \end{aligned}$$

with $M_i = hf_y(x_n + c_ih, Y_i)$, $i = 2, 3$ and

$$\begin{aligned} B &= 6(c_2 - c_3) + c_2(3c_3 - 2c_2)M_2 + c_3(2c_3 - 3c_2)M_3 \\ &\quad + c_2c_3(c_2 - c_3)M_2M_3. \end{aligned} \tag{4.19}$$

He shows that the order is generally 3 but if c_2 and c_3 are correlated,

$$c_3 = \frac{3 - 4c_2}{4 - 6c_2}, \tag{4.20}$$

the order becomes 4, a value which is usually attained only by four-stage versions of the standard type.

The new versions introduced in [74,75] share a common unusual feature: their b_i coefficients are equation dependent because they contain the Jacobian function; for systems of ODEs these become matrices. It follows that the coefficients must be updated at each step but this additional effort is largely compensated by the increased order and also, quite importantly, by massively better stability properties.

To illustrate the latter on the two-stage versions R and S we recall that the stability function of these versions is

$$R(\omega, z) = 1 + \omega[b_1^V + b_2^V] + \omega^2 a_{21}(z)b_2^V, \quad V = R, S$$

see [74], and also recall that the region of the three-dimensional $(\mathrm{Re}(\omega), \mathrm{Im}(\omega), z)$ space on which the inequality

$$|R(\omega, z)| < 1 \tag{4.21}$$

is satisfied is called a *region of stability* Ω for that method.

On Fig. 2 we take $c_2 = 2/3$ and show sections through the stability regions by planes $z = -1$ and $z = -4$ for S/R version on the left/right column. For the standard version a weak variation with z of stability area is seen but, as expected, a massive increase appears for the revised version.

For Ixaru's method, two pairs c_2, c_3 are of special importance with respect to stability because they give forth-order A-stable methods. These are $c_2 = 1/2$, $c_3 = 1$, and $c_2 = 1$, $c_3 = 1/2$. As a matter of fact, this is to our knowledge the first case when an explicit fourth-order method is A-stable.

To illustrate the influence of the stability properties in current runs, Ixaru takes the system:

$$\begin{aligned} y^{1'} &= (10\lambda + 9)y^1 - 10(\lambda + 1)y^2, \\ y^{2'} &= -9(\lambda + 1)y^1 - (9\lambda + 10)y^2, \\ x &\in [x_{\min} = 0, x_{\max} = 5], \qquad y^1(0) = y_0^1, \qquad y^2(0) = y_0^2, \end{aligned} \tag{4.22}$$

with the exact solution

$$\begin{aligned} y^1(x) &= 10(y_0^1 - y_0^2)\exp(\lambda x) + (-9y_0^1 + 10y_0^2)\exp(-x), \\ y^2(x) &= 9(y_0^1 - y_0^2)\exp(\lambda x) + (-9y_0^1 + 10y_0^2)\exp(-x). \end{aligned}$$

He uses $y_0^1 = y_0^2 = 1$ and $\lambda = -600$. The solution is then independent of λ: $y^1(x) = y^2(x) = \exp(-x)$, and if stability were not an issue the results at $h = 1/2$ or $1/4$ must be sufficiently accurate. However, this does not happen for all methods, as seen in Table 2 where relative errors in $y^1(x_{\max})$ are given for different stepwidths

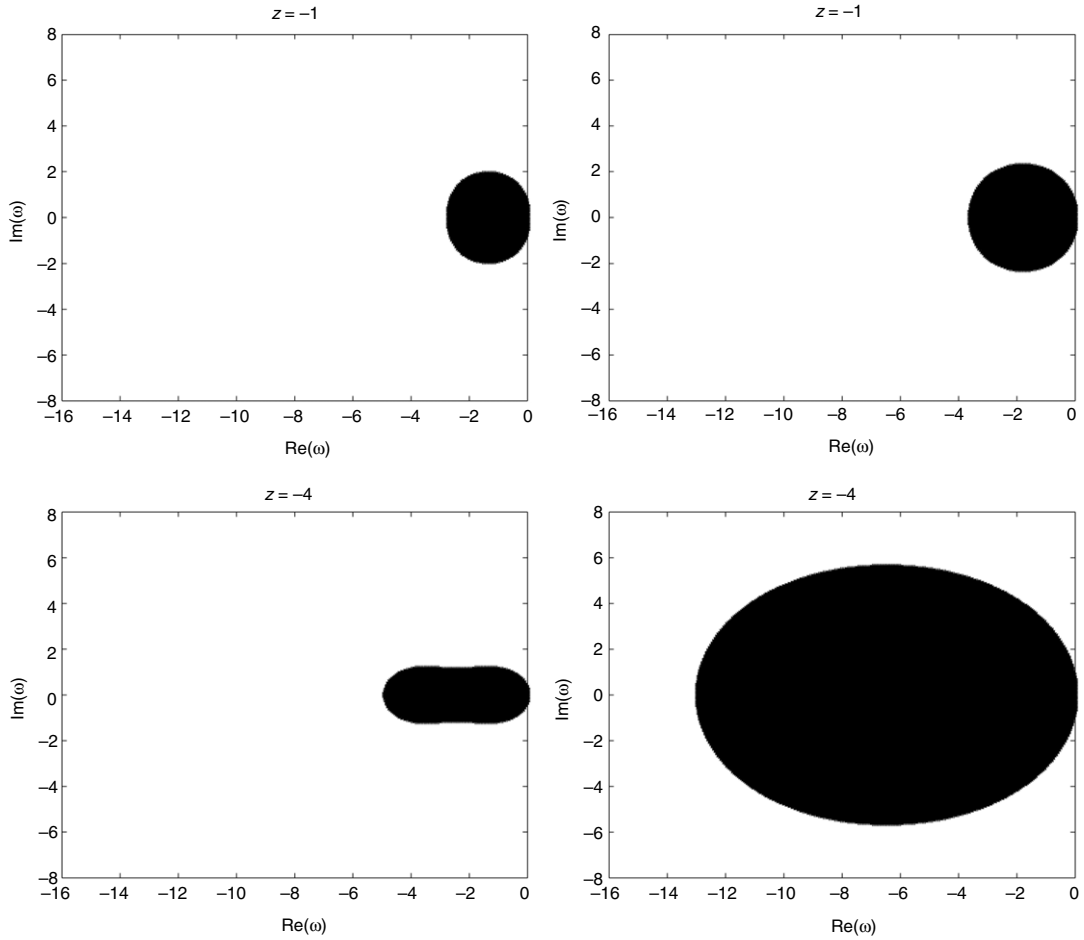

Fig. 2. Sections through the stability region by plane $z = const$ for fixed $c_2 = \frac{2}{3}$: standard version (left column), revised version (right column).

Table 2
Relative errors from the classical RK4 method and four versions of the fourth-order Ixaru method for the test system (4.22). Notation $a(b)$ means $a \times 10^b$.

h	RK4	Ixaru method			
		$c_2 = 1/8$	$c_2 = 1/4$	$c_2 = 3/8$	$c_2 = 1/2$
1/2	8.51(+57)	3.35(+13)	1.95(+10)	−2.11(+07)	−4.41(−04)
1/4	−7.82(+83)	−1.22(+35)	8.89(+26)	−1.51(+18)	−2.72(−05)
1/8	4.11(+216)	−9.67(+68)	−6.11(+51)	−4.76(+34)	−1.70(−06)
1/16	−NaN	−4.96(+113)	−1.27(+87)	−1.26(+53)	−1.06(−07)
1/32	−NaN	−8.54(+164)	−5.24(+108)	−7.15(+38)	−6.62(−09)
1/64	−NaN	−2.13(+127)	2.13(+28)	−4.34(−11)	−4.12(−10)
1/128	−NaN	2.71(−11)	1.25(−11)	−2.83(−12)	−2.55(−11)
1/256	−9.84(−12)	1.42(−12)	1.57(−12)	1.51(−13)	−1.13(−12)

(the relative errors in $y^2(x_{\max})$ have the same values) from the classical RK4 method, and from the Ixaru method with four values of c_2 (coefficients c_3 are correlated by (4.20)) approaching 1/2 closer and closer. It is seen that the alteration due to the instability is massive for the first method to lower down from the left to the right, up to a total extinction for the version with $c_2 = 1/2$ which is A-stable.

The examination of other methods in the same way appears as an interesting objective for the further research.

Appendix

Ixaru's functions $\eta_{-1}(Z), \eta_0(Z), \eta_1(Z), \ldots$, originally introduced in [14], are defined as follows:

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \le 0, \\ \cosh(Z^{1/2}) & \text{if } Z > 0, \end{cases} \tag{A.1}$$

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

while $\eta_m(Z)$ with $m > 0$ are further generated by recurrence

$$\eta_m(Z) = [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z, \quad m = 1, 2, 3, \ldots \tag{A.3}$$

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

$$\eta_m(0) = 1/(2m+1)!!, \quad m = 1, 2, 3, \ldots. \tag{A.4}$$

Some useful properties are as follows:

(i) Series expansion:

$$\eta_m(Z) = 2^m \sum_{q=0}^{\infty} \frac{(q+m)!}{q!(2q+2m+1)!} Z^q, \quad m = 0, 1, 3, \ldots. \tag{A.5}$$

(ii) Asymptotic behavior at large $|Z|$:

$$\eta_m(Z) \approx \begin{cases} \eta_{-1}(Z)/Z^{(m+1)/2} & \text{for odd } m, \\ \eta_0(Z)/Z^{m/2} & \text{for even } m. \end{cases} \tag{A.6}$$

(iii) Differentiation properties:

$$\eta_m'(Z) = \frac{1}{2}\eta_{m+1}(Z), \quad m = -1, 0, 1, 2, \ldots. \tag{A.7}$$

Good fortran routines for computing these functions exist, e.g. subroutine GEBASE in the CD attached to [1] or in code SLCPM12 from [16].

References

[1] L.Gr. Ixaru, G. Vanden Berghe, Exponential Fitting, Kluwer Academic Publishers, Dordrecht, 2004.
[2] L.Gr. Ixaru, Gazeta Matematica si Fizica, Seria B 51 (1960) 21.
[3] L.Gr. Ixaru, Canadian J. Phys. 49 (1971) 2947.
[4] L.Gr. Ixaru, An Algebraic Solution of the Schrödinger Equation, internal report IC/69/6, ICTP Trieste, 1969. http://streaming.ictp.it/preprints/P/69/006.pdf.
[5] L.Gr. Ixaru, The Algebraic Approach to the Scattering Problem, internal report IC/69/7, ICTP Trieste, 1969. http://streaming.ictp.it/preprints/P/69/007.pdf.
[6] L.Gr. Ixaru, J. Comput. Phys. 9 (1972) 159.
[7] L.Gr. Ixaru, Approximate Methods for Solving the Schrödinger Equation, Metode aproximative pentru rezolvarea ecuaţiei Schrödinger, Ph. D. Thesis, 1973 (unpublished).
[8] Gh. Adam, L.Gr. Ixaru, A. Corciovei, J. Comput. Phys. 22 (1976) 1.
[9] L.Gr. Ixaru, Gh. Adam, Rev. Roum. Phys. 24 (1979) 723.
[10] L.Gr. Ixaru, M.I. Cristu, M.S. Popa, J. Comput. Phys. 36 (1980) 170.
[11] L.Gr. Ixaru, J. Comput. Phys. 36 (1980) 182.
[12] L.Gr. Ixaru, Comput. Phys. Commun. 20 (1980) 97.
[13] L.Gr. Ixaru, Phys. Rev. D 25 (1982) 1557.
[14] L.Gr. Ixaru, Numerical Methods for Differential Equations, Reidel, Dordrecht–Boston–Lancaster, 1984.
[15] L.Gr. Ixaru, H. De Meyer, G. Vanden Berghe, J. Comput. Appl. Math. 88 (1998) 289.
[16] L.Gr. Ixaru, H. De Meyer, G. Vanden Berghe, Comput. Phys. Commun. 118 (1999) 259.
[17] L.Gr. Ixaru, Comput. Phys. Commun. 177 (2007) 897.
[18] L.Gr. Ixaru, Comput. Phys. Commun. 181 (2010) 1738.
[19] A.D. Raptis, A.C. Allison, Comput. Phys. Commun. 44 (1978) 95.
[20] T. Lyche, Numer. Math. 19 (1974) 65.
[21] L.Gr. Ixaru, M. Rizea, Comput. Phys. Commun. 19 (1980) 23.
[22] L.Gr. Ixaru, M. Rizea, J. Comput. Phys. 73 (1987) 306.
[23] J.P. Coleman, L.Gr. Ixaru, IMA J. Numer. Anal. 16 (1996) 179.
[24] J.P. Coleman, L.Gr. Ixaru, SIAM J. Numer. Anal. 44 (2006) 1441.
[25] L.Gr. Ixaru, Comput. Phys. Commun. 105 (1997) 1.
[26] L.Gr. Ixaru, H. De Meyer, G. Vanden Berghe, M. Van Daele, Comput. Phys. Commun. 100 (1997) 71.
[27] L.Gr. Ixaru, Comput. Phys. Commun. 147 (2002) 834.
[28] L.Gr. Ixaru, N.S. Scott, M.P. Scott, SIAM J. Sci. Comput. 28 (2006) 1252.
[29] W. Liniger, R.A. Willoughby, SIAM J. Numer. Anal. 7 (1970) 47.
[30] E. Stiefel, D.G. Bettis, Numer. Math. 13 (1969) 154.
[31] R.E. Greenwood, Ann. Math. Stat. 20 (1949) 608.
[32] P. Brock, F.J. Murray, Math. Tables Other Aids Comput. 6 (1952) 63 and 138.
[33] S.C.R. Dennis, Proc. Cambridge Phil. Soc. 65 (1960) 240.
[34] W. Gautschi, Numer. Math. 3 (1961) 381.
[35] H.E. Salzer, ZAMM 9 (1962) 403.
[36] N.S. Bakhvalov, L.G. Vasil'eva, USSR Comput. Math. Math. Phys. 8 (1969) 241.
[37] W. Gautschi, Math. Comp. 24 (1970).
[38] R. Piessens, ZAMM 50 (1970) 698.
[39] D. Levin, Math. Comp. 38 (1982) 531.
[40] G.A. Evans, J.R. Webster, Appl. Numer. Math. 23 (1997) 205.
[41] U.T. Ehrenmark, J. Comput. Appl. Math. 21 (1988) 87.
[42] G. Vanden Berghe, H. De Meyer, J. Vanthournout, J. Comput. Appl. Math. 31 (1990) 331.
[43] M. Van Daele, H. De Meyer, G. Vanden Berghe, Int. J. Comput. Math. 42 (1992) 83.
[44] H. De Meyer, J. Vanthournout, G. Vanden Berghe, J. Comput. Appl. Math. 30 (1990) 55.
[45] D. Hollevoet, M. Van Daele, G. Vanden Berghe, J. Comput. Appl. Math. 230 (2009) 260.
[46] Z. Wang, Comput. Phys. Commun. 171 (2005) 162.
[47] Z.A. Anastassi, T.E. Simos, Phys. Rep. -Rev. Sec. F Phys. Lett. 482 (2009) 1.
[48] H. Van De Vyver, J. Comput. Appl. Math. 188 (2006) 309.
[49] M. Calvo, M.J. Franco, J.I. Montijano, L. Randez, J. Comput. Appl. Math. 223 (2009) 387.
[50] H. Van de Vyver, Comput. Phys. Commun. 174 (2006) 255.
[51] H. Van de Vyver, ICNAAM 2005 Extended Abstrac, 2005, p. 566.
[52] L.Gr. Ixaru, B. Paternoster, J. Comput. Appl. Math. 106 (1999) 87.
[53] L.Gr. Ixaru, G. Vanden Berghe, H. De Meyer, J. Comput. Appl. Math. 140 (2002) 423.
[54] G. Vanden Berghe, L.Gr. Ixaru, H. De Meyer, J. Comput. Appl. Math. 132 (2001) 95.
[55] H. Van de Vyver, J. Comput. Appl. Math. 184 (2005) 442.
[56] J. Vigo-Aguiar, J. Martin-Vaquero, Appl. Math. Comput. 190 (2007) 80.
[57] G. Vanden Berghe, M. Van Daele, J. Comput. Appl. Math. 200 (2007) 140.
[58] T.E. Simos, Cent. Eur. J. Phys. 9 (2011) 1518.
[59] I. Alolyan, Z.A. Anastassi, T.E. Simos, Appl. Math. Comput. 218 (2012) 5370.
[60] I. Alolyan, T.E. Simos, J. Math. Chem. 49 (2011) 1843.
[61] D.S. Vlachos, Z.A. Anastassi, T.E. Simos, J. Math. Chem. 46 (2009) 1009.
[62] J. Vigo-Aguiar, T.E. Simos, Int. J. Quantum Chem. 103 (2005) 278.
[63] D. Conte, E. Esposito, B. Paternoster, L.Gr. Ixaru, Comput. Phys. Commun. 181 (2010) 128.
[64] K.J. Kim, R. Cools, L.Gr. Ixaru, J. Comput. Appl. Math. 140 (2002) 479.
[65] K.J. Kim, R. Cools, L.Gr. Ixaru, Appl. Numer. Math. 46 (2003) 59.
[66] K.J. Kim, Comput. Phys. Commun. 153 (2003) 135.
[67] L.Gr. Ixaru, B. Paternoster, Comput. Phys. Commun. 133 (2001) 177.
[68] K.J. Kim, J. Comput. Appl. Math. 174 (2005) 43.
[69] M. Van Daele, G. Vanden Berghe, H. Vande Vyver, Appl. Numer. Math. 53 (2005) 509.
[70] G.V. Milovanovic, A.S. Cvetkovic, M.P. Stanic, Appl. Math. Lett. 20 (2007) 853.
[71] A. Cardone, L.Gr. Ixaru, B. Paternoster, Numer. Algorithms 55 (2010) 467.
[72] K.J. Kim, C.S. Hoe, J. Comput. Phys. 205 (2007) 149.
[73] K.J. Kim, Appl. Math. Comput. 217 (2011) 7703.
[74] R. D'Ambrosio, L.Gr. Ixaru, B. Paternoster, Comp. Phys. Commun. 182 (2011) 322.
[75] L.Gr. Ixaru, Comput. Phys. Commun. 183 (2012) 63.
[76] J.C. Butcher, Numerical Methods for Ordinary Differential Equations, second ed., Wiley, Chichester, 2008.
[77] T.E. Simos, Comput. Phys. Comm. 115 (1998) 1.
[78] G. Vanden Berghe, H. De Meyer, M. Van Daele, T. Van Hecke, Comput. Phys. Comm. 123 (1999) 7.
[79] J.M. Franco, J. Comput. Appl. Math. 149 (2002) 407.
[80] G. Vanden Berghe, H. De Meyer, M. Van Daele, T. Van Hecke, J. Comput. Appl. Math. 125 (2000) 107.
[81] K. Ozawa, Japan J. Indust. Appl. Math. 16 (1999) 25.
[82] J.P. Coleman, Suzanne C. Duxbury, J. Comput. Appl. Math. 126 (2000) 47.
[83] B. Paternoster, Appl. Numer. Math. 28 (1998) 401.
[84] R. D'Ambrosio, M. Ferro, B. Paternoster, Math. Comput. Simul. 81 (2011) 1068.
[85] R. D'Ambrosio, E. Esposito, B. Paternoster, J. Comput. Appl. Math. 235 (2011) 4888.
[86] R. D'Ambrosio, E. Esposito, B. Paternoster, J. Math. Chem. 50 (1) (2012) 155–168.
[87] R. D'Ambrosio, E. Esposito, B. Paternoster, Appl. Math. Comput. (2012) http://dx.doi.org/10.1016/j.amc.2012.01.014.
[88] Y. Fang, Y. Song, X. Wu, Comput. Phys. Commun. 179 (2008) 801.
[89] J.M. Franco, J. Comput. Appl. Math. 187 (2006) 41.
[90] B. Paternoster, Appl. Numer. Math. 35 (2000) 339.
[91] B. Paternoster, in: P.M.A. Sloot, C.J.K. Tan, J.J. Dongarra, A.G. Hoekstra (Eds.), Computational Science—ICCS 2002, in: Lecture Notes in Computer Science, vol. 2331, Springer-Verlag, Amsterdam, 2002, pp. 459–466. Part III.
[92] B. Paternoster, in: P.M.A. Sloot, D. Abramson, A.V. Bogdanov, J.J. Dongarra, A.Y. Zomaya, Y.E. Gorbachev (Eds.), Computational Science—ICCS 2003, in: Lecture Notes in Computer Science, vol. 2658, Springer, Berlin, Heidelberg, 2003, pp. 131–138. Part II.
[93] H. Van de Vyver, Internat. J. Modern Phys. C 17 (5) (2006) 663.
[94] H. Van de Vyver, J. Comput. Appl. Math. 209 (2007) 33.
[95] B. Paternoster, in: V.N. Alexandrov, G.D. van Albada, P.M.A. Sloot, J.J.D ongarra (Eds.), Computational Science—ICCS 2003, in: Lecture Notes in Computer Science, vol. 3994, Springer-Verlag, 2006, pp. 700–707. Part IV.
[96] G. Vanden Berghe, M. Van Daele, Numer. Algorithms 46 (2007) 333.
[97] L.Gr. Ixaru, G. Vanden Berghe, H. De Meyer, Comput. Phys. Commun. 150 (2003) 116.
[98] J.D. Lambert, Numerical Methods for Ordinary Differential Systems: The Initial Value Problem, Wiley, Chichester, 1991.
[99] E. Hairer, S.P. Norsett, G. Wanner, Solving Ordinary Differential Equations I—Nonstiff Problems, in: Springer Series in Computational Mathematics, vol. 8, Springer-Verlag, Berlin, 2000.
[100] A. Paris, L. Randez, J. Comput. Appl. Math. 234 (2010) 767.
[101] H. Van de Vyver, New Astron. 11 (2006) 577.
[102] J. Vigo-Aguiar, J. Martin-Vaquero, Numer. Algorithms 48 (2008) 327.
[103] G. Vanden Berghe, M. Van Daele, H. Vande Vyver, J. Comput. Appl. Math. 159 (2003) 217.
[104] J.P. Coleman, J. Comput. Appl. Math. 92 (1998) 69.
[105] R. D'Ambrosio, M. Ferro, B. Paternoster, Appl. Math. Lett. 22 (2009) 1076.
[106] Z.A. Anastassi, T.E. Simos, J. Math. Chem. 41 (2007) 79.
[107] B. Paternoster, Int. J. Appl. Math. 6 (2001) 347.
[108] B. Paternoster, Rend. Mat. Appl. 23 (VII) (2003) 277.
[109] T.E. Simos, Appl. Math. Lett. 17 (2004) 601.
[110] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration, Structure-Preserving Algorithms for Ordinary Differential Equations, second ed., Springer-Verlag, Berlin, 2006.
[111] T.E. Simos, J. Vigo-Aguiar, Phys. Rev. E 67 (2003) 1.
[112] A. Tocino, J. Vigo-Aguiar, Math. Comput. Modelling 42 (2005) 873.
[113] J. Vigo-Aguiar, T.E. Simos, A. Tocino, Int. J. Mod. Phys. C 12 (2001) 225.
[114] H. Van de Vyver, New Astron. 10 (2005) 261.
[115] J.M. Franco, Comput. Phys. Commun. 177 (2007) 479.

[116] M. Calvo, M.J. Franco, J.I. Montijano, L. Randez, Comput. Phys. Commun. 178 (2008) 732.
[117] M. Calvo, M.J. Franco, J.I. Montijano, L. Randez, Comput. Phys. Commun. 181 (2010) 2044.
[118] G. Vanden Berghe, M. Van Daele, Numer. Algorithms 56 (2011) 591.
[119] M. Calvo, M.J. Franco, J.I. Montijano, L. Randez, J. Comput. Appl. Math. 218 (2008) 421.
[120] J.M. Franco, J. Comput. Appl. Math. 167 (2004) 1.