(Preprint for)

J. Álvarez and J. Rojo

An improved class of generalized Runge-Kutta methods for stiff problems. Part II: The separated system case

Appl. Math. Comput., 159 (2003), pp. 717-758

An improved class of generalized Runge-Kutta methods for stiff problems. Part II: The separated system case

Jorge Alvarez [a,1] and Jesús Rojo [a,1]

[a] *Departamento de Matemática Aplicada a la Ingeniería, E.T.S. de Ingenieros Industriales, Universidad de Valladolid, E-47011 Valladolid, Spain*
E-mail: joralv@wmatem.eis.uva.es, jesroj@wmatem.eis.uva.es

In order to study a generalization of the explicit p-stage Runge-Kutta methods, we introduce a new family of p-stage formulas for the numerical integration of some special systems of ODEs that provides better order and stability results with the same number of stages. In our recent paper entitled 'An improved class of generalized Runge-Kutta methods for stiff problems. Part I: The scalar case' we studied new schemes for the numerical integration of scalar autonomous ODEs. In this second part we will show that it is possible to generalize our GRK-methods so that they can be applied to some non-autonomous scalar ODEs and systems obtaining linearly implicit A-stable and L-stable methods. These methods do not require Jacobian evaluations in their implementation. Some numerical examples are discussed in order to show the good performance of the new schemes.

Key words: Generalized Runge-Kutta Methods, Stiff ODEs, Linear Stability, Numerical Experiments.

1 Introduction.

In our recent paper [7], first part of this work, we introduced the general form of a new class of explicit p-stage methods for the numerical integration of scalar autonomous ODEs. In the same paper, but also in [4,2,5], examples are shown of explicit two-stage methods of order three for the numerical integration of scalar autonomous ODEs, some of them being A-stable and L-stable.

[1] This work was partially supported by Programa Gral. de Apoyo a Proyectos de Investigación de la Junta de Castilla y León under proyect VA024/03 and by Programa C.I.C.Y.T under proyect BFM2002-03815.

Comparisons with Runge-Kutta methods as well as numerical experiments are also reported.

For brevity reasons, we refer to these methods as *GRK-methods* (Generalized Runge-Kutta methods). In what follows, we make this name also extensive to the methods for systems that we will study here.

Recently, in the Thesis of J. Álvarez [3] the GRK-methods (and the extension of these methods to 'separated' systems) have been introduced and studied in a systematic way, but the language used in this work is spanish, and so, it seems necessary to make the ideas of the Thesis available in an international journal. This is the main purpose of this paper.

We will study how the GRK-methods for scalar problems can be extended (with minor changes) in order to integrate more general problems. We will show that it is possible to obtain A-stable linearly implicit formulas for some non-autonomous scalar ODEs and systems. In [6] we presented a first two-stage third order method for separated systems of ODEs being L-stable, as well as preliminary results using our method to integrate systems that arise when solving some nonlinear parabolic PDEs by the method of lines approach.

Following this line, our aim is now to generalize this method by introducing the family of GRK-methods in order to obtain some properties that cannot be obtained from the classical explicit Runge-Kutta formulas. In fact, as we have seen when considering the scalar version of the GRK-methods (see [7]) the most important advantage of our methods is that we can obtain higher order with a reduced number of function evaluations. We will obtain linearly implicit methods of high order with important linear stability properties that cannot be obtained with the classical explicit Runge-Kutta methods. For example, it is possible to obtain order three and L-stability with only two stages (that is two function evaluations per integration step). This justifies the consideration of the formulas we will present here.

Our methods show also important advantages with respect to other classical implicit [9] and diagonally implicit [1] Runge-Kutta methods, and Rosenbrock type methods such as the ROW-methods (also called Rosenbrock-Wanner methods and modified Rosenbrock methods) [14,15,17] for which the exact Jacobian matrix must be evaluated at each step, because for our formulas the exact Jacobian matrix must not be computed when the methods are implemented.

Note at this point that, as we have remarked in [2], it is also possible to obtain two-stage third order formulas (belonging to the family of methods we will introduce) from any prefixed linear stability function. This can be of great interest when considering perturbed problems for which the exact solution of the unperturbed problem is known, because we can obtain methods specifically designed to integrate exactly the unperturbed problem.

As is well known, non autonomous systems can be easily formulated as autonomous systems, and so our treatment will consider only the autonomous case.

In the system case, that we are going to study here, we have that term s considered in [7] for the scalar case cannot be defined exactly in the same way because now the stages k_1 and k_2 are vectors. So, when considering this problem, we will see that the formula in [7] that gives us term s, must be modified into a formula that gives us term s as a square matrix with the same dimension of the system. Division by the vector k_1 has only sense when the vectorial function f defining the system

$$y' = f(y) \tag{1}$$

is of a special type that we will call 'separated' (and so the associated system is a 'separated system'). For this, as we will see later, function f must be given in the form (2). The special form of function f makes no available the GRK-methods for general systems. This limitation of the new methods is compensated by the important advantages of our methods (higher order, better linear stability properties, ...) when applied to the class of separated problems, with respect to classical methods such as Runge-Kutta formulas.

We have explored some important problems of practical interest for which our methods can be applied. As a result of this study, we have concluded that many important problems of interest that are formulated in terms of ODEs or PDEs can be solved with the formulas we will propose here. We also note that some non autonomous equations can be formulated in terms of an autonomous separated system and integrated with our methods.

When considering many important partial differential equations, and after a semi discretization (by using finite difference approximations) that transform these problems into a system of ordinary differential equations, we obtain separated systems for which our methods can be applied. For example, systems of this type appear when solving some parabolic partial differential equations by the method of lines. We will show examples of this later, by obtaining separated systems of ODEs from the Burgers' equation by the method of lines approach (with finite difference approximations in the spatial derivatives). In (20) we will show examples of this, and more precisely, we will consider as in [6] the problem studied in [11] (pp. 349–443) involving Burgers' equation.

When we observe the cases cited as practical in the literature we see that many of them are problems that we can solve with our methods. We can cite for example (26) (see [20] pp. 27 and [18]) and (28) (taken from [16], pp. 213) as interesting examples of this.

Following these ideas for scalar equations, we have adapted our methods in order to obtain formulas that can be applied to many second order differential equations of an special type. In [8] some preliminary results involving perturbed oscillators can be found.

As a resume, we will show clearly that the new methods can be applied to a wide class of problems considered of interest in the current literature. Also, for these problems for which the explicit (or linearly implicit) methods can be applied, we get very high orders of convergence and specially good linear stability properties for stiff problems that completely justifies the introduction of the new schemes and its study.

Now we can begin the description of the new formulas for separated systems.

2 The problem.

We will begin considering *separated* systems given by

$$\begin{aligned}
y'_{(1)} &= f_{11}(y_{(1)}) + f_{12}(y_{(2)}) + \ldots + f_{1m}(y_{(m)})\,,\\
y'_{(2)} &= f_{21}(y_{(1)}) + f_{22}(y_{(2)}) + \ldots + f_{2m}(y_{(m)})\,,\\
\vdots & \qquad\qquad \vdots\\
y'_{(m)} &= f_{m1}(y_{(1)}) + f_{m2}(y_{(2)}) + \ldots + f_{mm}(y_{(m)})\,,
\end{aligned} \tag{2}$$

that is, autonomous systems of ODEs $y' = f(y) = \sum_{j=1}^{m} F_j(y_{(j)})$ for which $f : \mathbb{R}^m \to \mathbb{R}^m$ is given by $f(y) = F(y)\mathbb{1}$, with $y = (y_{(1)}, y_{(2)}, \ldots, y_{(m)})$, $\mathbb{1} = (1, 1, \ldots, 1)^T$ and where F is the matrix

$$F(y) = \begin{pmatrix} f_{11}(y_{(1)}) & f_{12}(y_{(2)}) & \cdots & f_{1m}(y_{(m)}) \\ f_{21}(y_{(1)}) & f_{22}(y_{(2)}) & \cdots & f_{2m}(y_{(m)}) \\ \vdots & \vdots & & \vdots \\ f_{m1}(y_{(1)}) & f_{m2}(y_{(2)}) & \cdots & f_{mm}(y_{(m)}) \end{pmatrix}, \tag{3}$$

whose j-th column is given by F_j and with components $f_{ij} : \mathbb{R} \to \mathbb{R}$. Note that brackets are used for the components of vectors y and y'. These systems are thus given componentwise by

$$y'_{(i)} = f_i(y_{(1)}, y_{(2)}, \ldots, y_{(m)}) = \sum_{j=1}^{m} f_{ij}(y_{(j)})\,, \quad 1 \le i \le m\,. \tag{4}$$

Although the preceding expressions for the separated systems are not completely determined in an unique way because the additive constants can be assimilated to the components in many different ways, the methods we will introduce later give the same result independently of where we place these additive constants.

Note that we begin considering only (separated) autonomous systems of ODEs, but, as we will see later, some non autonomous systems that take the form $y'(x) = f(y(x)) + g(x)$ can be also integrated with the schemes we will introduce in this work. This can be easily seen by adding the trivial equation $x' = 1$ to the preceding non autonomous systems so that the resulting system takes an autonomous form. This resulting autonomous system is one dimension higher, and separated when $y'(x) = f(y(x))$ is separated. Our methods can be implemented for these non autonomous problems without increasing this dimension.

3 The new family of GRK-methods.

For problem (2), with initial condition $y(x_0) = y_0$ ($y_0 \in \mathbb{R}^m$), the general form of a p-stage method of our family is given by

$$y_{n+1} = y_n + hG_{p+1}(S_2, S_3, \ldots, S_p)\, k_1\,, \tag{5}$$

in terms of the stages

$$\begin{aligned} k_1 &= f(y_n) \\ k_2 &= f(y_n + hG_2\, k_1) \\ k_3 &= f(y_n + hG_3(S_2)\, k_1) \\ &\vdots \\ k_p &= f(y_n + hG_p(S_2, S_3, \ldots, S_{p-1})\, k_1)\,, \end{aligned} \tag{6}$$

where y_n, y_{n+1} and the k_i are m dimensional (column) vectors in $\mathbb{R}^m$ and where S_i and $G_i(S_2, S_3, \ldots, S_{i-1})$ are square matrices, that is $S_i \in M_{\mathbb{R}}(m)$ and $G_i(S_2, S_3, \ldots, S_{i-1}) \in M_{\mathbb{R}}(m)$ ($M_{\mathbb{R}}(m)$ is the space of m row square matrices with real elements). The matrices S_i take the form

$$\begin{pmatrix} \dfrac{f_{11}(y_{n(1)} + \alpha_1) - f_{11}(y_{n(1)})}{e_1\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1} & \cdots & \dfrac{f_{1m}(y_{n(m)} + \alpha_m) - f_{1m}(y_{n(m)})}{e_m\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1} \\ \vdots & & \vdots \\ \dfrac{f_{m1}(y_{n(1)} + \alpha_1) - f_{m1}(y_{n(1)})}{e_1\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1} & \cdots & \dfrac{f_{mm}(y_{n(m)} + \alpha_m) - f_{mm}(y_{n(m)})}{e_m\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1} \end{pmatrix}, \tag{7}$$

where $\alpha_j = h\, e_j\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1$ (with $1 \leq j \leq m$) and e_j is the m dimensional row vector in $\mathbb{R}^m$ whose components are all zero except for the

j-th component that takes the value 1. Note that the element in row p and column q (with $1 \le p, q \le m$) of the preceding matrix S_i is

$$\frac{f_{pq}(y_{n(q)} + h\, e_q\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1) - f_{pq}(y_{n(q)})}{e_q\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1}\,. \tag{8}$$

Stages k_i ($1 \le i \le p$) can be also given in terms of function F (see (3)) through relation

$$\begin{aligned} k_i &= F(y_n + h\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1)\mathbb{1} \\ &= \sum_{j=1}^{m} F_j(y_{n(j)} + h\, e_j\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1)\,, \end{aligned} \tag{9}$$

where $F_j(y_{n(j)} + h\, e_j\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1)$ is the j-th column of the square matrix $F(y_n + h\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1)$ given by

$$\begin{pmatrix} f_{11}(y_{n(1)} + h\, e_1\, G_i(*)\, k_1) & \cdots & f_{1m}(y_{n(m)} + h\, e_m\, G_i(*)\, k_1) \\ \vdots & & \vdots \\ f_{m1}(y_{n(1)} + h\, e_1\, G_i(*)\, k_1) & \cdots & f_{mm}(y_{n(m)} + h\, e_m\, G_i(*)\, k_1) \end{pmatrix}, \tag{10}$$

with $(*)$ denoting point $(S_2, S_3, \ldots, S_{p-1})$, and the element in row p and column q (with $1 \le p, q \le m$) of this matrix given by

$$f_{pq}(y_{n(q)} + h\, e_q\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1)\,. \tag{11}$$

Now it is easily seen that the j-th column of matrices S_i in (7) takes the form

$$\frac{F_j(y_{n(j)} + h\, e_j\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1) - F_j(y_{n(j)})}{e_j\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1}, \tag{12}$$

and is therefore given in terms of the j-th column of stage k_i (see (9)) minus the j-th column of stage k_1 and divided by the term $e_j\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1$ taken from the argument of the j-th column of stage k_i.

From the preceding comments it is now clear that matrices S_i can be seen as a generalization (together with a minor modification) of the terms s_i considered in the scalar case. In fact, it is not difficult to see that the family of methods introduced in [7] for scalar problems can also be formulated in this manner, but we will not do that here.

Note that matrices S_i for this kind of systems can be seen as approximations to $hf_y(y_n)$, that is, approximations to the Jacobian matrix of function f evaluated in y_n (and scaled by the step h). This follows from the fact that (8) can be considered an approximation to the partial derivative of the p-th component of function f with respect to his q-th variable at point y_n. In fact, for this kind of systems we have

$$\frac{\partial f_p}{\partial y_{(q)}}(y_n) = \frac{\partial f_{pq}}{\partial y_{(q)}}(y_{n(q)}) \approx \frac{f_{pq}(y_{n(q)} + h\,\delta_q) - f_{pq}(y_{n(q)})}{h\,\delta_q}\,, \tag{13}$$

with $\delta_q = e_q\, G_i(S_2, S_3, \ldots, S_{i-1})\, k_1$.

From our last observation we can conclude that our GRK-methods are similar to the Rosenbrock methods [19] and other related formulae such as the W-methods [22], the MROW-methods [24] and the generalized Runge-Kutta methods [23] for which the exact Jacobian matrix must not be computed when methods are implemented. In [11] some of this methods can be found.

The most important advantage of our GRK-methods with respect to these methods is that for our formulas it is not necessary to make new evaluations of function f to obtain the approximate Jacobian matrix. This is so because matrices S_i (from which we have the approximations to the Jacobian matrix) are obtained from the information contained in the stages k_i with no extra evaluations of function f (at the only cost of working with square matrices during the evaluations).

As we have commented before, separated systems are not completely determined because of additive constants. More precisely, taking in (2) $\tilde{f}_{ij} = f_{ij} + c_{ij}$ in place of f_{ij} $(1 \le i, j \le m)$ with c_{ij} given constants satisfying $\sum_{j=1}^{m} c_{ij} = 0$ for $i = 1, 2, \ldots, m$, we get the same system. It is a simple task to show that when we apply any of our methods to both separated systems (representing the same system) $y' = f(y)$ and $y' = \tilde{f}(y)$, taking the same initial value and the same stepsize, we obtain the same result.

4 A first two-stage GRK-method for separated systems.

Before studying in detail the new family of methods, we begin considering a first example of a two-stage formula. Note that function G_2 in (6) is constant, that is, $G_2 = c_2 I$ where c_2 is a constant and I is the identity matrix in $M_{\mathbb{R}}(m)$. Therefore, a two-stage method for systems from the preceding family of schemes takes the form

$$y_{n+1} = y_n + h\, G_3(S_2)\, k_1\,, \tag{14}$$

where the stages are

$$k_1 = f(y_n)\,, \quad k_2 = f(y_n + h c_2 k_1)\,, \tag{15}$$

and S_2 is the matrix

$$\begin{pmatrix} \frac{f_{11}(y_{n(1)}+hc_2e_1k_1)-f_{11}(y_{n(1)})}{c_2e_1k_1} & \cdots & \frac{f_{1m}(y_{n(m)}+hc_2e_mk_1)-f_{1m}(y_{n(m)})}{c_2e_mk_1} \\ \vdots & & \vdots \\ \frac{f_{m1}(y_{n(1)}+hc_2e_1k_1)-f_{m1}(y_{n(1)})}{c_2e_1k_1} & \cdots & \frac{f_{mm}(y_{n(m)}+hc_2e_mk_1)-f_{mm}(y_{n(m)})}{c_2e_mk_1} \end{pmatrix} \quad (16)$$

The formula is completely determined from the values of c_2 and function G_3.

From Butcher's theory we know that a Runge-Kutta method of order q for scalar problems can show order less than q when applied to systems of ODEs. However, for $q \leq 3$ any Runge-Kutta method of order q for scalar autonomous problems shows the same order when applied to systems of ODEs (see for example [16] pp. 173-175 for more details). For our methods this result also holds, that is, for $q \leq 3$ any GRK-method of order q for scalar autonomous problems shows the same order when applied to separated systems of ODEs.

As a first example we will obtain an L-stable formula. In order to attain L-stability we must take G_3 given by a rational function whose denominator must be interpreted in terms of inverse matrices (note that the argument S_2 of function G_3 is a square matrix). We look for a function $G_3(s)$ whose denominator takes the form $(1-a\,s)^\alpha$, that is, $G_3(S_2)$ in (14) is given by $(I-a\,S_2)^{-\alpha}\,N(S_2)$ where $\alpha \in \mathbb{N}$, $a \in \mathbb{R}$ is a constant and N is a polynomial function (as before, I stands for the identity matrix). We take function G_3 in this manner so that only one LU factorization must be done for each integration step. Taking the values $\alpha = 3$, $c_2 = 2/3$, a as the root of polynomial $6x^3 - 18x^2 + 9x - 1 = 0$ given by

$$\begin{aligned} a &= 1 + \frac{\sqrt{6}}{2}\sin\left(\frac{1}{3}\arctan\left(\frac{\sqrt{2}}{4}\right)\right) - \frac{\sqrt{2}}{2}\cos\left(\frac{1}{3}\arctan\left(\frac{\sqrt{2}}{4}\right)\right) \\ &\approx 0.435866521508459\,, \end{aligned} \quad (17)$$

and function G_3 in (14) given by

$$G_3(S_2) = (I - a\,S_2)^{-3}\left(I + \frac{1-6a}{2}\,S_2 + \frac{1-9a+18a^2}{6}\,S_2^2\right)\,, \quad (18)$$

we obtain a two-stage third order L-stable method for separated systems whose associated stability function takes the form

$$R(z) = \frac{2 + 2\,(1-3a)\,z + (1-6a+6a^2)\,z^2}{2\,(1-a\,z)^3}\,, \quad (19)$$

with a given by (17).

For more details involving the L-stability that we get from the preceding stability function $R(z)$, [11] pp. 96–98 is a good reference. In [6] this method is obtained with slightly different notations.

5 A first numerical experiment with systems.

As a first example, in order to show the good performance of the preceding method, we will consider a numerical experiment involving the Burgers' equation

$$u_t + u\, u_x = \nu\, u_{xx} \quad \text{or equivalently} \quad u_t + \left(\frac{u^2}{2}\right)_x = \nu\, u_{xx}\,, \quad \nu > 0\,, \tag{20}$$

where $u = u(x,t)$ and we take $0 \le x \le 1$ and $0 \le t \le 1$. Initial and Dirichlet boundary conditions for our example are taken as

$$u(x,0) = (\text{sen}(3\pi x))^2 \cdot (1-x)^{3/2}\,, \qquad u(0,t) = u(1,t) = 0\,. \tag{21}$$

The preceding nonlinear parabolic problem is taken from [11] (see pp. 349 and 443) and was originally designed by Burgers in 1948 as a mathematical model illustrating the theory of turbulence. Nowadays it remains interesting as a nonlinear equation resembling the Navier-Stokes equations in fluid dynamics. Note that for small values of ν the solution possesses shock waves and for $\nu \to 0$ we obtain discontinuous solutions. Note also that Burgers' equation can be considered as an example of hyperbolic problem with artificial diffusion for small ν.

Now we will apply the method of lines to this equation as follows. We will consider a uniform mesh along the x-axis and replace all spatial derivatives in the right equation of (20) by centered finite difference approximations. Taking

$$\Delta x = \frac{1}{N+1}\,, \qquad u_i(t) = u(i\Delta x, t) \qquad i = 0, 1, \ldots, N+1\,, \tag{22}$$

we get a separated system of ODEs for this method of lines approach to Burgers' equation, that is given by

$$\begin{aligned} u_i' &= -\frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x} + \nu \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}\,, \qquad i = 1, 2, \ldots, N \\ u_i(0) &= (\text{sen}(3\pi i \Delta x))^2 \cdot (1 - i\Delta x)^{3/2}\,, \qquad i = 1, 2, \ldots, N\,, \end{aligned} \tag{23}$$

with $u_i = u_i(t)$. From the boundary conditions we get that $u_0(t) = u_{N+1}(t) = 0$ must hold. Obviously our method can be applied to the this separated system. After the appropriate exclusions and substitutions we can note by inspection that the Jacobian matrix associated to this system is tridiagonal.

In [6] we have applied our method with fixed stepsize $h = 0.04$ to the preceding system taking $N = 24$ and $\nu = 0.2$ and obtaining in this way the numerical solution (see the first figure in [6]). For these values the system becomes banded of dimension 24 and the associated Jacobian matrix is tridiagonal. The problem is mildly stiff with the eigenvalues of the Jacobian belonging to interval $[-499, -1]$ (the dominant eigenvalue being close to -498) for the integration interval considered.

With fixed stepsize $h = 2^{-k}$ for the values $k = 2, 3, \ldots, 10$ over 2^k steps, the value of the numerical solution (for $t = 1$) was also computed in [6] by using our method, and the magnitude of the error E (measured in the Euclidean norm of the space $\mathrm{I\!R}^{24}$) for the different stepsizes considered can be found in the second figure of this work. The exact solution at the specified output point was computed very carefully taking fixed stepsize $h = 0.0001$. In the double logarithmic scale used for that figure, the error is closely represented by a straight line whose slope equals the order of the method. Figure shows clearly the order three of our method, in complete agreement with our theoretical result.

In the following sections we will repeat this numerical experiment with other third and fourth order methods.

To complete this first approach to our methods for separated systems we will also consider the following numerical experiments.

6 Some interesting numerical experiments.

We will study the family of problems taken from [13], pp. 34 (see also [21], pp. 233 and [12]).

$$\begin{aligned} y_1' &= -(b + an)y_1 + by_2^n \qquad & y_1(0) &= c^n \\ y_2' &= y_1 - ay_2 - y_2^n & y_2(0) &= c \end{aligned} \tag{24}$$

whose solution is given by

$$y_1(x) = c^n e^{-anx}, \quad y_2(x) = ce^{-ax}. \tag{25}$$

We take the values $a = 0.1$, $c = 1$, $n = 4$ and $b = 100^i$ $(i = 0, 1, 2, 3)$ in the interval $0 \le x \le 10$. The problem is stiffer for great values of parameter b. In fact, the eigenvalues along the exact solution satisfy $\lambda_1 \approx -b$ and $\lambda_2 \approx -a$). The nonlinear character of the problems depends on the value n (the problem is more nonlinear when n is great). For more details on this problem see [13].

With fixed stepsize $h = 2^{-k}$ for $k = 0, 1, 2, \ldots, 10$ we integrate along $10 \cdot 2^k$ steps obtaining in this way approximations to the exact solution y (for $x = 10$) with our two-stage method. The magnitude of the global error E (in the Euclidean norm) for the different stepsizes h and for each of the problems considered is shown in Figure 1 in double logarithmic scale. It can be seen that the method shows order less than three (in fact two) when applied to this problem taking $b = 1000000$ (marked in figure with crosses) and $b = 10000$ (circles) for the range of stepsizes we are considering here. Taking $b = 100$ (diamonds) the order goes from two to three when the stepsize is reduced. The order reduction can be explained in terms of the so called B-convergence and many implicit methods also show this behaviour when applied to some nonlinear stiff ODEs. Finally, taking $b = 1$ (squares) the problem is no longer stiff and our method shows order three as expected.

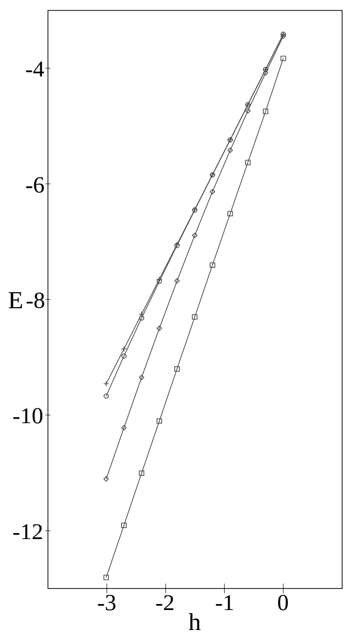

Fig. 1. Error as a function of the stepsize in double logarithmic scale for our method (autonomous problem).

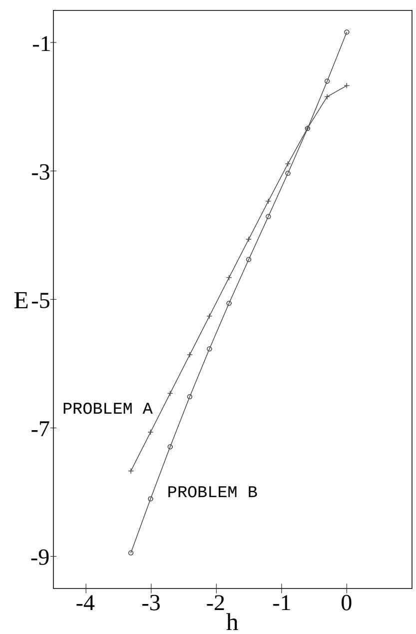

Fig. 2. Error as a function of the stepsize in double logarithmic scale for our method (non autonomous problems).

Now we will consider two non autonomous stiff problems. Problem A is taken from [20], pp. 27 and is given by

$$y' = -10^6\, y + \cos x + 10^6 \sin x\,, \quad y(0) = 1\,, \tag{26}$$

with solution

$$y(x) = \sin x + e^{-10^6\, x}\,. \tag{27}$$

Note that this problem can be considered as part of the family of scalar equations proposed by Prothero and Robinson in [18].

Problem B is given in terms of the following non autonomous system

$$\begin{aligned} y_1' &= -2\,y_1 + y_2 + 2\sin x & \qquad y_1(0) &= 2 \\ y_2' &= 998\,y_1 - 999\,y_2 + 999(\cos x - \sin x) & \qquad y_2(0) &= 3 \end{aligned} \tag{28}$$

taken from [16], pp. 213, for which the exact solution takes the form

$$y_1(x) = 2e^{-x} + \sin x\,, \quad y_2(x) = 2e^{-x} + \cos x\,. \tag{29}$$

Both problems are stiff (the eigenvalue for problem A is $\lambda = -1000000$ and for problem B the eigenvalues are $\lambda_1 = -1$ and $\lambda_2 = -1000$). We apply our two-stage method to both problems with fixed stepsizes $h = 2^{-k}$ for $k = 0, 1, 2, \ldots, 11$ over $10 \cdot 2^k$ steps. Figure 2 shows the global error E (in the Euclidean norm) as a function of the stepsize h in double logarithmic scale. As in the previous example, we can observe that the order that shows our method when applied to problem A is nearly two (for the range of stepsizes considered here). Taking small enough stepsizes the order changes from two to three as expected. For problem B the order changes from two to three when the stepsize is reduced, as can be seen in the figure. As we have pointed before, this can be explained in terms of the concept of B-convergence.

7 Order conditions for the two-stage methods.

As we have shown in the preceding numerical experiments, it is possible to obtain two-stage methods of order three for separated systems. In fact, in this case, the order conditions (for order three) are the same we obtained considering scalar autonomous problems. In the same way as when we considered the scalar case, it suffices to obtain the order conditions for the polynomial type methods, because from these conditions we easily obtain those of the general formulas.

Also as in the scalar case, two-stage methods of polynomial type (for systems) can be defined as follows

$$y_{n+1} = y_n + hG_3(S_2)\,k_1\,, \tag{30}$$

where the stages are given by

$$k_1 = f(y_n)\,, \quad k_2 = f(y_n + hc_2k_1)\,, \tag{31}$$

S_2 is the matrix

$$\begin{pmatrix} \frac{f_{11}(y_{n(1)}+hc_2e_1k_1)-f_{11}(y_{n(1)})}{c_2e_1k_1} \cdots \frac{f_{1m}(y_{n(m)}+hc_2e_mk_1)-f_{1m}(y_{n(m)})}{c_2e_mk_1} \\ \vdots \qquad\qquad\qquad\qquad\qquad \vdots \\ \frac{f_{m1}(y_{n(1)}+hc_2e_1k_1)-f_{m1}(y_{n(1)})}{c_2e_1k_1} \cdots \frac{f_{mm}(y_{n(m)}+hc_2e_mk_1)-f_{mm}(y_{n(m)})}{c_2e_mk_1} \end{pmatrix} \tag{32}$$

and where function G_3 is given in terms of S_2 by

$$G_3(S_2) = c_3 \left(I + \sum_{i=1}^{r_3} a_i S_2^i \right), \qquad r_3 \in \mathbb{N}, \tag{33}$$

where I stands for the identity matrix of dimension m. Order conditions (for order three) are the same as those given for scalar autonomous problems (see [7]), that is

$$c_3 = 1, \tag{34}$$

$$c_3a_1 = 1/2, \tag{35}$$

$$c_3c_2a_1 = 1/3, \tag{36}$$

$$c_3a_2 = 1/6. \tag{37}$$

After solving this conditions for order three, we deduce that $c_2 = 2/3$ and that function G_3 associated to any third order method of polynomial type can be given in the form

$$G_3(S_2) = I + \frac{1}{2}S_2 + \frac{1}{6}S_2^2 + \sum_{i=3}^{r_3} a_i S_2^i, \qquad r_3 \in \mathbb{N}, \tag{38}$$

where the free parameters a_i (with $i \geq 3$) can be arbitrarily chosen.

Additional conditions for order four are now different from those associated to the scalar case (see again [7]). In fact, now we have four additional order conditions (one more than in scalar case) that are given by

$$c_3c_2^2a_1 = 1/4, \tag{39}$$

$$c_3c_2a_2 = 1/12, \tag{40}$$

$$c_3c_2a_2 = 1/4, \tag{41}$$

$$c_3a_3 = 1/24, \tag{42}$$

and two of these conditions ((40) and (41)) cannot be satisfied at the same time. It is easily seen that first three equations are not satisfied for the values of the parameters that we must take so that the two-stage method has order three, and therefore it is not possible to obtain formulas of order four with only two stages (as in scalar case). However, we can satisfy the fourth equation taking $a_3 = 1/24$ in such a way that the principal part of the local truncation error (PPLTE) is minimized. For this choice of parameter a_3, and taking also $a_1 = 1/2$, $a_2 = 1/6$, $c_2 = 2/3$ and $c_3 = 1$ (to attain order three), the resulting formulas show order four when applied to lineal problems with constant coefficients.

Now, order conditions for two-stage methods for separated systems given in terms of rational type functions, are easily obtained from those obtained for polynomial type formulas, following the same ideas as in scalar case. A two-stage method of rational type for systems is given (generalizing the associated methods for scalar case) by formulas (30)–(32), where function G_3 in terms of S_2 takes the form

$$G_3(S_2) = c_3 \left(I + \sum_{i=1}^{d_3^*} d_i S_2^i \right)^{-1} \left(I + \sum_{i=1}^{n_3^*} n_i S_2^i \right) , \qquad n_3^*, d_3^* \in \mathbb{N} , \tag{43}$$

As in the scalar case, it suffices to take $G_2 = c_2 I$ with $c_2 = 2/3$ and function G_3 given by (43) with a Taylor's expansion in powers of S_2 of the form

$$G_3(S_2) = I + \frac{1}{2} S_2 + \frac{1}{6} S_2^2 + O(S_2^3) . \tag{44}$$

Therefore, it is enough to take the values $n_3^* = d_3^* = 2$ in (43) in order to obtain the order conditions for order three methods of rational type from those of polynomial type. We easily obtain in this way the fourth order conditions

$$\begin{aligned} c_2 &= 2/3 , && (45) \\ c_3 &= 1 , && (46) \\ n_1 &= 1/2 + d_1 , && (47) \\ n_2 &= 1/6 + (1/2) d_1 + d_2 , && (48) \end{aligned}$$

as in the scalar case (see [7]).

If we also want to minimize the principal part of the local truncation error, we must take $n_3^* = d_3^* = 3$ in (43) and expand in (44) to one higher order obtaining the additional condition

$$n_3 = 1/24 + (1/6) d_1 + (1/2) d_2 + d_3 . \tag{49}$$

From the preceding considerations we deduce that the general form of a two-stage third order method of rational type for systems is

$$y_{n+1} = y_n + h G_3(S_2)\, k_1 , \tag{50}$$

where stages are given by

$$k_1 = f(y_n)\,, \quad k_2 = f\left(y_n + \frac{2}{3}hk_1\right)\,, \tag{51}$$

matrix S_2 takes the form

$$\begin{pmatrix} \frac{f_{11}\left(y_{n(1)}+\frac{2}{3}he_1k_1\right)-f_{11}(y_{n(1)})}{\frac{2}{3}e_1k_1} & \cdots & \frac{f_{1m}\left(y_{n(m)}+\frac{2}{3}he_mk_1\right)-f_{1m}(y_{n(m)})}{\frac{2}{3}e_mk_1} \\ \vdots & & \vdots \\ \frac{f_{m1}\left(y_{n(1)}+\frac{2}{3}he_1k_1\right)-f_{m1}(y_{n(1)})}{\frac{2}{3}e_1k_1} & \cdots & \frac{f_{mm}\left(y_{n(m)}+\frac{2}{3}he_mk_1\right)-f_{mm}(y_{n(m)})}{\frac{2}{3}e_mk_1} \end{pmatrix} \tag{52}$$

and function G_3 is

$$\begin{aligned} G_3(S_2) = & \left(I + d_1S_2 + d_2S_2^2 + \sum_{i=3}^{d_3^*} d_iS_2^i\right)^{-1} \\ & \cdot \left(I + \frac{1+2d_1}{2}S_2 + \frac{1+3d_1+6d_2}{6}S_2^2 + \sum_{i=3}^{n_3^*} n_iS_2^i\right)\,. \end{aligned} \tag{53}$$

The general form of a two-stage third order method of rational type for systems that minimizes the principal part of the local truncation error is given by formulas (50–52), where now function G_3 takes the form

$$\begin{aligned} G_3(S_2) = & \left(I + d_1S_2 + d_2S_2^2 + d_3S_2^3 + \sum_{i=4}^{d_3^*} d_iS_2^i\right)^{-1} \\ & \cdot \left(I + \frac{1+2d_1}{2}\,S_2 + \frac{1+3d_1+6d_2}{6}\,S_2^2 \right. \\ & \left. + \frac{1+4d_1+12d_2+24d_3}{24}\,S_2^3 + \sum_{i=4}^{n_3^*} n_iS_2^i\right)\,. \end{aligned} \tag{54}$$

8 Order conditions for the three-stage methods.

Now situation changes with respect to the two-stage case. First, definition of matrix S_3 that we will introduce later changes with respect to scalar case. Also, since two matrices S_2 and S_3 appear now in definition, non commutativity of products of those matrices must be taken into account. These makes the new three-stage formulas for systems more complicated than two-stage methods (only one matrix appears in this case).

We begin considering the general form of the three-stage methods for separated systems that we can obtain from Section 3 taking $p=3$. We have

$$y_{n+1} = y_n + hG_4(S_2, S_3)\, k_1\,, \tag{55}$$

where y_n, y_{n+1} and k_1 are vectors in $\mathbb{R}^m$ and S_i are square matrices of dimension m.

Stages k_i (with $1 \le i \le 3$) are given by

$$\begin{aligned} k_1 &= f(y_n) \\ k_2 &= f(y_n + hG_2\, k_1) \\ k_3 &= f(y_n + hG_3(S_2)\, k_1)\,, \end{aligned} \tag{56}$$

(with $G_2 = c_2 I$) in terms of the square matrices S_2 given in (16) and S_3 given by

$$\begin{pmatrix} \dfrac{f_{11}(y_{n(1)}+\alpha_1) - f_{11}(y_{n(1)})}{e_1 G_3(S_2)\, k_1} & \cdots & \dfrac{f_{1m}(y_{n(m)}+\alpha_m) - f_{1m}(y_{n(m)})}{e_m G_3(S_2)\, k_1} \\ \vdots & & \vdots \\ \dfrac{f_{m1}(y_{n(1)}+\alpha_1) - f_{m1}(y_{n(1)})}{e_1 G_3(S_2)\, k_1} & \cdots & \dfrac{f_{mm}(y_{n(m)}+\alpha_m) - f_{mm}(y_{n(m)})}{e_m G_3(S_2)\, k_1} \end{pmatrix}, \tag{57}$$

where $\alpha_j = he_j G_3(S_2)\, k_1$ (with $1 \le j \le m$) and e_j stands for the vector in $\mathbb{R}^m$ with all null components except the j-th that is 1. Note that the element in row p and column q (with $1 \le p, q \le m$) in matrix S_3 is given by

$$\frac{f_{pq}(y_{n(q)} + he_q G_3(S_2)\, k_1) - f_{pq}(y_{n(q)})}{e_q G_3(S_2)\, k_1}\,. \tag{58}$$

Obviously $G_i\, k_1$ stands for the product of matrix G_i and vector k_1.

We will begin obtaining the order conditions for the three-stage methods of polynomial type, that is, for those methods for which the associated functions G_2, G_3 and G_4 are polynomial functions. More precisely, $G_2 = c_2 I$ (with c_2 a given constant) and the other functions given in the form

$$\begin{aligned} G_3(S_2) &= c_3 \left(I + \sum_{i=1}^{r_3} a_{3,\,2\,2\,\cdots\,2}\, S_2^i \right), \quad r_3 \in \mathbb{N}\,, \\ G_4(S_2, S_3) &= c_4 \left(I + \sum_{i=1}^{r_4^*} a^*_{4,\,\sigma_1\,\sigma_2\,\cdots\,\sigma_i}\, S_{\sigma_1} S_{\sigma_2} \cdots S_{\sigma_i} \right), \quad r_4^* \in \mathbb{N}\,, \end{aligned} \tag{59}$$

where the coefficients $a_{3,\,2\,2\,\cdots\,2}$ of the first sum in (59) play a similar role as the coefficients a_i in the scalar case and in the two-stage methods for separated systems we have seen before. Any of the subscripts σ_k that appears in the second sum of (59) can take the values 2 or 3. We introduce this kind of new subscripts σ_k because of the possible non commutativity of products with matrices S_2 and S_3 (we must differentiate the coefficients of the products of these matrices even if the same factors appear in the product but in different order).

As we have commented in scalar case, only some of the free parameters will appear in order conditions (because S_2 and S_3 are $O(h)$). However, the resulting order conditions are too complicated and therefore we will define a new matrix $\tilde{S}_3$ that will substitute matrix S_3 in order to simplify the following study. We will take $\tilde{S}_3 = S_3 - S_2$ so that $\tilde{S}_3 = O(h^2)$ holds, and in this way the number of parameters that will appear in the order conditions is less than before and the order conditions are simplified. After introducing $\tilde{S}_3$, the three-stage methods of polynomial type can be rewritten as follows

$$y_{n+1} = y_n + h\tilde{G}_4(S_2, \tilde{S}_3)\, k_1\,, \tag{60}$$

where $\tilde{S}_3 = S_3 - S_2$, with S_2 and S_3 defined as before in terms of the stages given in (56) and where now

$$\tilde{G}_4(S_2, \tilde{S}_3) = c_4 \left(I + \sum_{i=1}^{r_4} a_{4,\sigma_1\sigma_2\cdots\sigma_i}\, S_{\sigma_1} S_{\sigma_2} \cdots S_{\sigma_i} \right)\,, \quad r_4 \in \mathbb{N}\,, \tag{61}$$

(functions G_2 and G_3 are given as before). Subscripts σ_k that appear in the sum of (61) can take the values 2 and 3. We will take $S_{\sigma_k} = S_2$ when $\sigma_k = 2$ and $S_{\sigma_k} = \tilde{S}_3$ when $\sigma_k = 3$. From the fact that $S_2 = O(h)$ and $\tilde{S}_3 = O(h^2)$, we can note that in the sum of (61) it suffices to consider those subscripts for which $n_2 + 2\,n_3 \leq r_4$, where n_2 stands for the number of subscripts σ_k (from coefficient $a_{4,\sigma_1\sigma_2\cdots\sigma_i}$) that take the value 2 and n_3 stands for the number of subscripts σ_k that take the value 3. So in sum only appear those terms (and the associated coefficients) that also appear in the order conditions for order less or equal than $r_4 + 1$.

We will show that now it is not possible to obtain fifth order methods with only three stages, that is, the situation changes with respect to scalar case. However it is possible to obtain order four and to retain the remaining good linear stability properties observed in scalar case. Moreover, as we will see later, it is possible to satisfy nearly all the order conditions for order five, and therefore the resulting methods behave as fifth order formulas when applied to some problems.

To obtain order five it suffices to take $r_3 = 2$ in (59) and $r_4 = 4$ in (61), and the resulting order conditions are completely given in terms of the parameters c_i $(2 \leq i \leq 4)$, $a_{3,2}$, $a_{3,22}$ and $a_{4,\sigma_1\sigma_2\cdots\sigma_i}$ (with $n_2 + 2\,n_3 \leq 4$).

The order conditions that a three-stage method of polynomial type must satisfy in order to be a fifth order formula are given by

$$c_4 = 1, \tag{62}$$
$$c_4 a_{4,2} = 1/2, \tag{63}$$
$$c_4 \left(c_2(a_{4,2} - a_{4,3}) + c_3 a_{4,3}\right) = 1/3, \tag{64}$$
$$c_4 a_{4,22} = 1/6, \tag{65}$$
$$c_4 \left(c_2^2(a_{4,2} - a_{4,3}) + c_3^2 a_{4,3}\right) = 1/4, \tag{66}$$
$$c_4 \left(c_2(a_{4,22} - a_{4,23}) + c_3 a_{4,23}\right) = 1/12, \tag{67}$$
$$c_4 \left(c_2(a_{4,22} - a_{4,32}) + c_3(a_{4,32} + a_{3,2}a_{4,3})\right) = 1/4, \tag{68}$$
$$c_4 a_{4,222} = 1/24, \tag{69}$$
$$c_4 \left(c_2^3(a_{4,2} - a_{4,3}) + c_3^3 a_{4,3}\right) = 1/5, \tag{70}$$
$$c_4 \left(c_2^2(a_{4,22} - a_{4,32}) + c_3^2(a_{4,32} + 2a_{3,2}a_{4,3})\right) = 3/10, \tag{71}$$
$$c_4 \left(c_2^2(a_{4,22} - a_{4,23}) + c_3^2 a_{4,23}\right) = 1/20, \tag{72}$$
$$\begin{aligned} c_4 \Big(c_2^2&(a_{4,22} - a_{4,23} - a_{4,32} + a_{4,33}) \\ &+c_2c_3(a_{4,23} + a_{4,32} - 2a_{4,33} + a_{3,2}a_{4,3}) + c_3^2 a_{4,33}\Big) = 2/15, \end{aligned} \tag{73}$$
$$c_4 \left(c_2(a_{4,222} - a_{4,322}) + c_3(a_{4,322} + a_{3,22}a_{4,3})\right) = 1/15, \tag{74}$$
$$c_4 c_3 a_{3,2} a_{4,32} = 1/20, \tag{75}$$
$$c_4 \left(c_2(a_{4,222} - a_{4,232} + c_3(a_{4,232} + a_{3,2}a_{4,23})\right) = 1/20, \tag{76}$$
$$c_4 \left(c_2(a_{4,222} - a_{4,223} + c_3 a_{4,223}\right) = 1/60, \tag{77}$$
$$c_4 a_{4,2222} = 1/120. \tag{78}$$

It is easy to check that all these conditions cannot be satisfied at the same time, but it is possible to satisfy nearly all of them. Therefore, we cannot obtain any three-stage fifth order formula for separated systems. However, we can obtain an infinite family of three-stage fourth order methods solving conditions (62–69). We make it as follows:

Step 1. From (62) we have that $c_4 = 1$ (that is the consistency condition). After substituting this value in the remaining equations we get directly the values of coefficients $a_{4,2}$, $a_{4,22}$ and $a_{4,222}$ from equations (63), (65) and (69).

Step 2. Substituting these values in the rest of equations and solving the non linear system given by equations (64) and (66) we get the values of c_2 and $a_{4,3}$ in terms of parameter c_3

Step 3. Finally we obtain coefficients $a_{4,23}$ and $a_{3,2}$ from equations (67) and (68) in terms of the parameters c_3 and $a_{4,32}$).

We obtain in this way the following solution

$$c_2 = \frac{3-4c_3}{2\,(2-3c_3)}\,, \quad c_4 = 1\,, \quad a_{4,2} = \frac{1}{2}\,, \quad a_{4,22} = \frac{1}{6}\,, \quad a_{4,222} = \frac{1}{24}\,,$$

$$
\begin{aligned}
a_{3,2} &= \frac{(9-39c_3+58c_3^2-30c_3^3)+(54-288c_3+600c_3^2-576c_3^3+216c_3^4)a_{4,32}}{2c_3\,(2-3c_3)}\,,\\
a_{4,3} &= \frac{1}{6\,(3-8c_3+6c_3^2)}\,, \quad a_{4,23} = \frac{1-c_3}{6\,(3-8c_3+6c_3^2)}\,.
\end{aligned} \tag{79}
$$

The remaining parameters can be arbitrarily chosen.

Additional conditions for order five are given by equations (70–78) and most of them can be satisfied. In fact, it is possible to satisfy all of them except for one (equations (71) and (75) cannot be satisfied at the same time). For this end we can follow the steps:

Step 1. We substitute the values (79) (obtained solving the fourth order conditions) in the nine additional conditions for order five. After this, conditions (70) and (72) give the same equation. We therefore obtain a nonlinear system of eight equations in eight unknowns (the remaining parameters) that has no solution.

Step 2. We directly obtain two values for coefficient c_3 that satisfy equation (70) (that is the same as equation (72) after the preceding substitution) and one value for $a_{4,2222}$ from equation (78).

Step 3. After substituting the calculated values in the preceding step it is now possible to obtain directly coefficients $a_{4,33}$ and $a_{4,223}$ from equations (73) and (77) respectively. It can be also observed that equations (71) and (75) cannot be satisfied at the same time because both depend on parameter $a_{4,32}$. We satisfy the first of these equations (obviously it is also possible to satisfy the second one obtaining two different values for coefficient $a_{4,32}$).

Step 4. Finally, after substituting the calculated values, we get the remaining coefficients $a_{3,22}$ and $a_{4,232}$ from equations (74) and (76) ($a_{3,22}$ is given in terms of the free parameter $a_{4,322}$).

The values of the coefficients we obtain in this way are

$$
\begin{aligned}
c_2 &= \frac{6\mp\sqrt{6}}{10}\,, \quad c_3 = \frac{6\pm\sqrt{6}}{10}\,, \quad c_4 = 1\,, \quad a_{3,2} = \frac{-3\pm 2\sqrt{6}}{5}\,,\\
a_{3,22} &= \frac{(17+144\,a_{4,322})\mp(3+96\,a_{4,322})\sqrt{6}}{50}\,, \quad a_{4,2} = \frac{1}{2}\,,\\
a_{4,3} &= \frac{9\pm\sqrt{6}}{36}\,, \quad a_{4,22} = \frac{1}{6}\,, \quad a_{4,23} = \frac{6\mp\sqrt{6}}{72}\,, \quad a_{4,32} = \frac{-1\pm\sqrt{6}}{8}\,,\\
a_{4,33} &= \frac{1\pm 4\sqrt{6}}{72}\,, \quad a_{4,222} = \frac{1}{24}\,, \quad a_{4,232} = \frac{-3\pm 2\sqrt{6}}{48}\,,\\
a_{4,223} &= \frac{3\mp\sqrt{6}}{144}\,, \quad a_{4,2222} = \frac{1}{120}\,.
\end{aligned} \tag{80}
$$

Parameter $a_{4,322}$ and the rest of parameters that do not appear in order five conditions can be arbitrarily chosen.

Satisfying at step 3 equation (75) (in place of equation (71)) the solution we obtained in (80) is only modified in the values of coefficients $a_{3,2}$, $a_{4,32}$ and $a_{4,232}$, that must be replaced by the values

$$a_{3,2} = \frac{\pm\sqrt{6}}{5}\,, \quad a_{4,32} = \frac{-1\pm\sqrt{6}}{12}\,, \quad a_{4,232} = \frac{-1\pm\sqrt{6}}{48}\,, \tag{81}$$

or

$$a_{3,2} = \frac{6\mp 2\sqrt{6}}{5}\,, \quad a_{4,32} = \frac{4\pm\sqrt{6}}{24}\,, \quad a_{4,232} = \frac{5\mp\sqrt{6}}{48}\,, \tag{82}$$

because at this case we have two different values for coefficient $a_{4,32}$ (for each of the obtained solutions).

In what follows we will study the rational case. A three-stage method of rational type for systems is given (with the notations introduced in polynomial case) by an expression like the considered in (60), that is

$$y_{n+1} = y_n + h\tilde{G}_4(S_2, \tilde{S}_3)\, k_1\,. \tag{83}$$

The stages k_1, k_2 and k_3 are given as in the polynomial case (see (56)), and so are also given the matrices S_2 and $\tilde{S}_3$ (see (16) and (57)). However, functions G_3 and $\tilde{G}_4$ are now given by

$$\begin{aligned} G_3(S_2) &= c_3 \left(I + \sum_{i=1}^{d_3^*} d_{3,\,2\,2\cdots 2}\, S_2^i \right)^{-1} \left(I + \sum_{i=1}^{n_3^*} n_{3,\,2\,2\cdots 2}\, S_2^i \right)\,, \\ \tilde{G}_4(S_2,\tilde{S}_3) &= c_4 \left(I + \sum_{i=1}^{d_4^*} d_{4,\,\sigma_1\,\sigma_2\cdots\sigma_i}\, S_{\sigma_1} S_{\sigma_2} \cdots S_{\sigma_i} \right)^{-1} \\ &\quad \cdot \left(I + \sum_{i=1}^{n_4^*} n_{4,\,\sigma_1\,\sigma_2\cdots\sigma_i}\, S_{\sigma_1} S_{\sigma_2} \cdots S_{\sigma_i} \right)\,. \end{aligned} \tag{84}$$

Function G_2, as before, is given by $G_2 = c_2 I$ (with c_2 a given constant).

Remember that subscripts σ_k in (84) can take the values 2 or 3 and we take $S_{\sigma_k} = S_2$ when $\sigma_k = 2$ and $S_{\sigma_k} = \tilde{S}_3$ when $\sigma_k = 3$. Remember also that in the sums of (84) defining $\tilde{G}_4$ we only will consider these addends of the sum for which $n_2 + 2\,n_3 \le d_4^*$ in the first sum and $n_2 + 2\,n_3 \le n_4^*$ in the second sum holds (here n_2 is the number of subscripts for which $\sigma_k = 2$ and n_3 the number of subscripts for which $\sigma_k = 3$).

Now we are going to study the order conditions for the three-stage methods of rational type. As we have seen before (when considering the scalar case and the two-stage methods for systems) we will obtain these order conditions from those obtained in the polynomial case. However, the possible non commutativity of the products must be now taken into account.

We begin considering the fourth order conditions for the polynomial type methods that are given as we have seen by the system of equations (62–69) and whose solution is given in (79). After determining the coefficients for the three-stage fourth order methods of polynomial type it suffices to equal functions G_2, G_3 and $\tilde{G}_4$ associated to the rational methods with those associated to the polynomial formulas to the adequate order. It is not difficult to see that it is enough to take $n_3^* = d_3^* = 1$ and $n_4^* = d_4^* = 3$ in (84).

Equaling we obtain that G_2 is given as in the polynomial case, that is, $G_2 = c_2 I$ with the constant c_2 given in terms of the free parameter c_3 as we have seen in (79). Comparing functions G_3 and $\tilde{G}_4$ defined by (84) with the corresponding to the polynomial case we get that parameter c_3 can be arbitrarily chosen and that we must take $c_4 = 1$. The remaining coefficients in the definition of function G_3 are given in terms of those calculated in polynomial case (see (79)) through relations

$$n_{3,2} = d_{3,2} + a_{3,2}\,, \tag{85}$$
$$n_{4,2} = d_{4,2} + a_{4,2}\,, \tag{86}$$
$$n_{4,3} = d_{4,3} + a_{4,3}\,, \tag{87}$$
$$n_{4,22} = d_{4,22} + a_{4,2}\, d_{4,2} + a_{4,22}\,, \tag{88}$$
$$n_{4,23} = d_{4,23} + a_{4,3}\, d_{4,2} + a_{4,23}\,, \tag{89}$$
$$n_{4,32} = d_{4,32} + a_{4,2}\, d_{4,3} + a_{4,32}\,, \tag{90}$$
$$n_{4,222} = d_{4,222} + a_{4,2}\, d_{4,22} + a_{4,22}\, d_{4,2} + a_{4,222}\,. \tag{91}$$

Note that we must substitute coefficients given in (79) in these formulas (we do not make it here for simplicity).

To minimize the principal part of the local truncation error in such a way that as many as possible order five conditions are satisfied (in fact all except for one as we have seen in polynomial case), it suffices to take $n_3^* = d_3^* = 2$ and $n_4^* = d_4^* = 4$ in (84). So we obtain that coefficients c_i (with $2 \leq i \leq 4$) are given as in (80) and that the following relations must hold

$$n_{3,2} = d_{3,2} + a_{3,2}\,, \tag{92}$$
$$n_{3,22} = d_{3,22} + a_{3,2}\, d_{3,2} + a_{3,22}\,, \tag{93}$$
$$n_{4,2} = d_{4,2} + a_{4,2}\,, \tag{94}$$
$$n_{4,3} = d_{4,3} + a_{4,3}\,, \tag{95}$$
$$n_{4,22} = d_{4,22} + a_{4,2}\, d_{4,2} + a_{4,22}\,, \tag{96}$$
$$n_{4,23} = d_{4,23} + a_{4,3}\, d_{4,2} + a_{4,23}\,, \tag{97}$$

$$
\begin{aligned}
n_{4,32} &= d_{4,32} + a_{4,2}\, d_{4,3} + a_{4,32}\,, & (98)\\
n_{4,33} &= d_{4,33} + a_{4,3}\, d_{4,3} + a_{4,33}\,, & (99)\\
n_{4,222} &= d_{4,222} + a_{4,2}\, d_{4,22} + a_{4,22}\, d_{4,2} + a_{4,222}\,, & (100)\\
n_{4,223} &= d_{4,223} + a_{4,3}\, d_{4,22} + a_{4,23}\, d_{4,2} + a_{4,223}\,, & (101)\\
n_{4,232} &= d_{4,232} + a_{4,2}\, d_{4,23} + a_{4,32}\, d_{4,2} + a_{4,232}\,, & (102)\\
n_{4,322} &= d_{4,322} + a_{4,2}\, d_{4,32} + a_{4,22}\, d_{4,3} + a_{4,322}\,, & (103)\\
n_{4,2222} &= d_{4,2222} + a_{4,2}\, d_{4,222} + a_{4,22}\, d_{4,22} + a_{4,222}\, d_{4,2} + a_{4,2222}\,. & (104)
\end{aligned}
$$

In the preceding relations we must substitute coefficients (80) (modified and completed if desired with (81) and (82)).

9 Linear stability function of the methods for systems.

The study of the linear stability properties of the methods for systems is now more complicated that in scalar autonomous case. This is so because when studying formulas for separated systems we must consider in place of the test equation $y' = \lambda\, y$ with $\lambda \in \mathbb{C}$, the system test $y' = A\, y$ where A is a square matrix of dimension m with m different eigenvalues $\lambda_i \in \mathbb{C}$ $(1 \le i \le m)$ with negative real parts. With the preceding conditions we know that the exact solution to this system tends to zero when x tends to infinity and that there exists a non singular matrix Q with $Q^{-1} A\, Q = \Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_m]$. The transformation $y = Q\, z$ enables us to simplify the study of the linear stability properties of our methods. In fact, this study is reduced to consider the scalar test equation because the system test and the difference formulas defining our methods are uncoupled with the preceding transformation. In order to see that this is so it suffices to apply any p-stage method for systems (given by (5–7)) to the system test $y' = A\, y$ (satisfying all the above mentioned conditions) obtaining in this way

$$
y_{n+1} = y_n + hG_{p+1}(S_2, S_3, \ldots, S_p)\, k_1\,, \tag{105}
$$

where now the stages k_i are given recursively by

$$
\begin{aligned}
k_1 &= A\, y_n\\
k_2 &= A\,(I + hG_2\, A)\, y_n\\
k_3 &= A\,(I + hG_3(hA)\, A)\, y_n\\
&\;\vdots\\
k_p &= A\,(I + hG_p(hA, hA, \ldots, hA)\, A)\, y_n\,,
\end{aligned} \tag{106}
$$

because, applied to the system, the square matrices S_i satisfy $S_i = h\, A$ (for $i = 2, 3, \ldots, p$).

We now define $y_n = Q\,w_n$ and $k_i = Q\,\alpha_i$ (for $i = 1, 2, \ldots, p$), that is we apply the transformation to uncouple the system. After multiplying by Q^{-1} relations (105) and (106) and making the preceding transformation (remembering that $Q^{-1}A\,Q = \Lambda$) we get

$$w_{n+1} = w_n + hG_{p+1}(h\Lambda, h\Lambda, \ldots, h\Lambda))\,\alpha_1\,, \tag{107}$$

with the stages given recursively by

$$\begin{aligned}
\alpha_1 &= \Lambda\,w_n \\
\alpha_2 &= \Lambda\,(I + hG_2\,\Lambda)\,w_n \\
\alpha_3 &= \Lambda\,(I + hG_3(h\Lambda)\,\Lambda)\,w_n \\
&\;\;\vdots \\
\alpha_p &= \Lambda\,(I + hG_p(h\Lambda, h\Lambda, \ldots, h\Lambda)\,\Lambda)\,w_n\,,
\end{aligned} \tag{108}$$

as can be easily seen observing that relation $Q^{-1}G_i(hA, hA, \ldots, hA)\,A\,Q = G_i(h\Lambda, h\Lambda, \ldots, h\Lambda)\,\Lambda$ holds.

We have seen in this way that the difference systems defining our methods (when applied to the test system) are uncoupled with the transformation $y = Q\,w$, and obviously the system test is also uncoupled to the form $w' = \Lambda\,w$ by this transformation. For this reason, in what follows it suffices to consider the scalar test equation given by $y' = \lambda y$ with $\lambda \in \mathbb{C}$ and $\Re(\lambda) < 0$, when studying the linear stability properties of the methods for separated systems.

When we apply a p-stage method for systems defined by (5–7) to the scalar test equation, we obtain

$$y_{n+1} = R(z)\,y_n\,, \tag{109}$$

where $R(z)$ is the linear stability function associated, with $z = h\lambda$. From (5–7) we obtain recursively

$$\begin{aligned}
k_1 &= \lambda\,y_n \\
S_2 &= z \\
S_3 &= z \\
&\;\;\vdots \\
S_p &= z\,,
\end{aligned} \tag{110}$$

and therefore the linear stability function takes the form

$$R(z) = 1 + z\,G_{p+1}(z, z, \ldots, z)\,. \tag{111}$$

Note that with the modification in the definition of matrices S_i (by including functions G_i) with respect to scalar case, the linear stability function is now given in a more simple form than in the similar expression given in [7].

At this point we also note that with the modification introduced when studying the three-stage methods for separated systems by introducing the matrix term $\tilde{S}_3 = S_3 - S_2$, we have from (110) that $\tilde{S}_3 = 0$ (when method is applied to scalar test equation). Therefore the linear stability function is given in this case by $R(z) = 1 + z\,\tilde{G}_4(z,0)$, as can be deduced from (60).

10 A first example of L-stable three-stage method of order four.

We have seen before an example of L-stable two-stage method of order three for separated systems, together with some numerical experiments to illustrate the good performance of this formula when applied to different stiff problems.

We also obtained the general form for the three-stage methods of order four for separated systems. Obviously most of these methods are not interesting because of the high computational cost associated. However, many of the methods perform well in many problems because of the high order obtained an the good linear stability properties (the formulas contain approximations to the Jacobian matrix with no additional function evaluations). To reduce the computational cost associated we will only consider those formulas for which only one LU factorization per step is necessary. We also will look for methods with good linear stability properties such as A-stability and L-stability, in order to obtain formulas that perform well when applied to stiff problems.

In what follows we are going to see a first example of a three-stage L-stable method of order four for separated systems. We look for methods whose associated linear stability function is a rational function with only one real pole (so that only one LU factorization per integration step is necessary) as occurs, for example, with the SDIRK methods. It is not difficult to see that to obtain an order four L-stable method, whose linear stability function has an unique real pole, the multiplicity of this pole must be greater or equal than four. There exists only one real value of the pole that enable us to obtain the preceding properties with multiplicity four, and this value is given by the root of polynomial

$$24\,x^4 - 96\,x^3 + 72\,x^2 - 16\,x + 1\,, \tag{112}$$

that takes approximately the value $a \approx 0.57281606$ (see [11], pp. 96–98 for more details). The corresponding linear stability function is the rational function $R(z)$ with numerator of degree three and denominator of degree four, that is given in terms of the preceding value a by

$$R(z) = \frac{6+6(1-4a)z+3(1-8a+12a^2)z^2+(1-12a+36a^2-24a^3)z^3}{6\,(1-a\,z)^4}\,. \tag{113}$$

We can obtain a method satisfying all the above requirements as follows:

Step 1. We take the following values for the free parameters $a_{4,32}$ and c_3 in (79)

$$a_{4,32} = 0\,, \quad c_3 = \frac{6+\sqrt{6}}{10}\,. \tag{114}$$

Note that the value we are taking for c_3 is the same we obtained for three-stage fifth order methods in scalar case.

Step 2. We substitute these values in (79) and the so obtained solution (that assures order four for the three-stage methods of polynomial type) in relations (85–91). We obtain in this way a family of three-stage fourth order methods of rational type. Note that any of these formulas is completely determined from the values of the coefficients d_*.

Step 3. Finally, between all these many options that we have in order to obtain a method with the desired linear stability function, we take this obtained by making zero the following coefficients

$$d_{4,3} = d_{4,23} = d_{4,32} = 0\,, \tag{115}$$

and taking

$$d_{3,2} = -a\,, \tag{116}$$

we obtain in terms of the above mentioned value a the solution

$$\begin{gathered}
c_2 = \frac{6-\sqrt{6}}{10}\,, \quad c_3 = \frac{6+\sqrt{6}}{10}\,, \quad c_4 = 1\,, \quad d_{3,2} = -a\,, \\
d_{4,2} = -4\,a\,, \quad d_{4,3} = 0\,, \quad d_{4,22} = 6\,a^2\,, \quad d_{4,23} = 0\,, \quad d_{4,32} = 0\,, \\
d_{4,222} = -4\,a^3\,, \quad d_{4,2222} = a^4\,, \quad n_{3,2} = \frac{(6-5\,a)-\sqrt{6}}{5}\,, \\
n_{4,2} = \frac{1-8\,a}{2}\,, \quad n_{4,3} = \frac{9+\sqrt{6}}{36}\,, \quad n_{4,22} = \frac{36\,a^2-12\,a+1}{6}\,, \\
n_{4,23} = \frac{6\,(1-12\,a)-(1+8\,a)\sqrt{6}}{72}\,, \quad n_{4,32} = 0\,, \\
n_{4,222} = \frac{-96\,a^3+72\,a^2-16\,a+1}{24}\,.
\end{gathered} \tag{117}$$

The remaining parameters are taken equal to zero.

Note that in the preceding formula we have introduced the coefficient $d_{4,2222}$ that do not appear in fourth order conditions. We make it because, as we have commented before, to obtain L-stability the denominator in the associated linear stability function (113) must be of degree four.

Now we will briefly comment why we make zero the coefficients in (115). We make zero the coefficients d_* in (115) corresponding to those terms with at least one the factor $\tilde{S}_3$, that is, the coefficient has at least one 3 in the subscript. We make this so that when making the LU factorization only the matrix S_2 appears.

We have taken the parameter $d_{3,2} = -a$ in (116) so that no additional LU factorizations are necessary to calculate the stages (in fact stage k_3). It seems better to reduce the computational cost associated with the method by making zero coefficient $d_{3,2}$ in (116), but different numerical experiments show that with this choice for the parameter the errors grow when integrating many stiff problems with moderate stepsizes h.

Note at this point that the three-stage fourth order L-stable formula we have obtained (and other formulas we can obtain in a similar way) performs better, with respect to number of function evaluations per integration step, than SDIRK methods of Runge-Kutta type. In [11], pp. 98 it is shown that at least four stages are necessary to obtain a SDIRK formula of order four and L-stable.

In what follows, we will illustrate with some numerical experiments the performance of the obtained L-stable formula.

11 Some numerical experiments with stiff problems.

We now repeat the numerical experiments of the preceding sections with our new three-stage fourth order L-stable method.

When we apply this method to the ODE system associated to Burgers' equation (by the MOL approach) that we described in (23), taking the values $N = 24$ and $\nu = 0.2$ and integrating with fixed stepsize $h = 0.04$, we obtain the Figure 3 for the numerical solution. This figure is very similar to Figure 1 obtained in [6] for the two-stage third order method.

In Figure 4 we show, in double logarithmic scale, the error E (in the Euclidean norm in $\mathbb{R}^{24}$) at point $t = 1$ that we obtain integrating with fixed stepsize $h = 2^{-k}$ for $k = 2, 3, \ldots, 10$ the preceding problem. When comparing this figure with the Figure 2 obtained in [6] for the two-stage third order method,

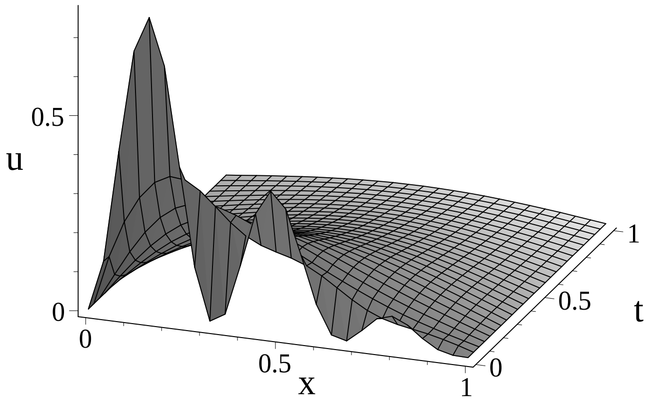

Fig. 3. Numerical solution: MOL approach to Burgers' equation taking $\nu = 0.2$, $N = 24$ and $h = 0.04$.

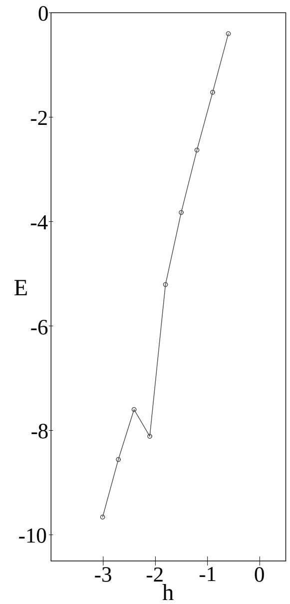

Fig. 4. Error as a function of stepsize (double logarithmic scale) for our method.

we can note that for great values of the stepsize h the order three formula performs slightly better than the fourth order one. However, when reducing the stepsize h the fourth order formula performs much better than the third order one as expected.

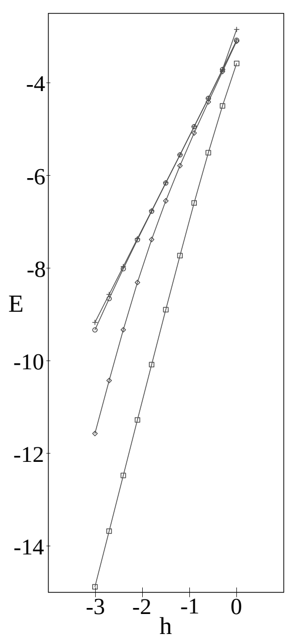

Fig. 5. Error as a function of the stepsize in double logarithmic scale for our method (autonomous problem).

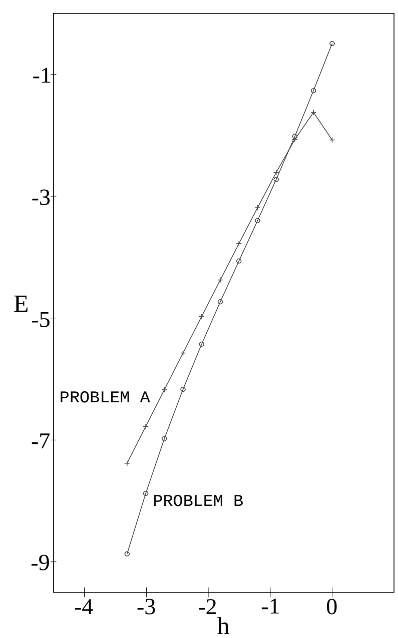

Fig. 6. Error as a function of the stepsize in double logarithmic scale for our method (non autonomous problems).

In Figure 5 we show in double logarithmic scale the error E (for $x = 10$) in the

Euclidean norm, we obtain when integrating along $10 \cdot 2^k$ steps problem (24) with fixed stepsizes $h = 2^{-k}$ for $k = 0, 1, \ldots, 10$. The values for the parameters in this problem are taken as for the two-stage third order method in a preceding numerical experiment (for comparison purposes). So we can compare the new results with those obtained for the two-stage method (see Figure 1). It can be observed (comparing the figures) that for the values $b = 1000000$ (crosses in the figure) and $b = 10000$ (circles) we obtain similar results with both methods. In both cases, for the range of stepsizes considered, we can observe that the order seems to be nearly two (lower than the expected order). Taking $b = 100$ (diamonds) we see in Figure 5 that the order grows from two to four when the stepsize is reduced and that the error is lower than the obtained with the two-stage method. As we have pointed out before, this observed reduction of the order is related with the concept of B-convergence and many implicit methods show also this behaviour when applied to some non linear stiff differential equations. Finally, for the value $b = 1$ (squares) problem is not stiff and our fourth order method gives a numerical approximation to the exact solution much better than those obtained with the two-stage formula.

We also repeat the numerical experiments with problems A and B (see (26) and (28) respectively) and the obtained results are shown in Figure 6 . Comparing this figure with Figure 2 obtained for the third order method, we can observe that in both problems we obtain similar results with the two methods for the range of stepsizes considered.

12 Some other A-stable and L-stable methods of two and three stages.

In preceding sections we have obtained two L-stable methods for separated systems and now we will give some other methods in order to complete our study.

From the general form of the two-stage third order methods of rational type for separated systems (see 50–53) we will now obtain an A-stable formula. We begin considering a function $G_3(S_2)$ of the form $(I - a\, S_2)^{-2}\, N(S_2)$ for a certain constant $a \in \mathbb{R}$ and a certain polynomial function N of degree two, so that only one LU factorization will be necessary per integration step. In order to obtain a method of order three, we must take in (53) the values $d_1 = -2\, a$ and $d_2 = a^2$ (the remaining parameters are taken $n_i = d_i = 0$ for $i \geq 3$). Now it suffices to obtain the value of constant a so that the resulting formula becomes A-stable. Remembering that, as we have seen in a preceding section, the linear stability function R associated to the method is given by $R(z) = 1 + z\, G_3(z)$, we obtain

$$R(z) = \frac{6 + 6\,(1-2a)\,z + 3\,(1-4a+2a^2)\,z^2 + (1-6a+6a^2)\,z^3}{6\,(1-a\,z)^2}\,, \quad (118)$$

and we get the value of constant a making zero the coefficient of z^3 in the numerator of (118), that is, solving equation $1-6a+6a^2=0$. From the two different values we obtain in this way we have that the one for A-stability is given by

$$a = \frac{3+\sqrt{3}}{6} \approx 0.78867513\,. \quad (119)$$

For more details related to the A-stability associated to the above function $R(z)$, the book [11] pp. 97 is again a good reference. Summarizing, the values of the parameters we must take in order to obtain the A-stable two-stage third order method for separated systems are given by

$$c_2 = \frac{2}{3}, \quad c_3 = 1, \quad d_1 = -\frac{3+\sqrt{3}}{3}, \quad d_2 = \frac{2+\sqrt{3}}{6}, \quad n_1 = -\frac{3+2\sqrt{3}}{6}. \quad (120)$$

We now are going to see how to obtain a L-stable two-stage third order method of rational type for systems that minimizes the principal part of the local truncation error. To this end we begin considering the general form (50–52), but where now function G_3 takes the form (54), from which we can conclude that the method satisfies all the required properties except for the L-stability. As for other methods obtained previously, we take function $G_3(S_2)$ of the form $(I - a\,S_2)^{-4}\,N(S_2)$ for a certain constant $a \in \mathbb{R}$ and a certain polynomial function N of degree three. This moves us to take in (54) the values $d_1 = -4\,a$, $d_2 = 6\,a^2$, $d_3 = -4\,a^3$ and $d_4 = a^4$ (the remaining parameters d_i take the value zero and $n_i = 0$ for $i \geq 4$). The value of the constant a is determined in such a way that the resulting formula is L-stable. Making zero the coefficient of z^4 in the numerator of the linear stability function $R(z)$, it is easy to check that we obtain the following linear stability function

$$R(z) = \frac{6+6(1-4a)z+3(1-8a+12a^2)z^2+(1-12a+36a^2-24a^3)z^3}{6\,(1-a\,z)^4}\,, \quad (121)$$

for the resulting L-stable method, in terms of the value of a that is given as the root of polynomial $1-16\,a+72\,a^2-96\,a^3+24\,a^4=0$ that takes approximately the value

$$a \approx 0.57281606\,. \quad (122)$$

In [11], pp. 98 we can find this value of a for the L-stability. Note that the value of a in (122) is the same that we obtained in Section 10 for the three-stage fourth order L-stable formula. Moreover, the linear stability function associated to this three-stage method (see (113)) and to the last two-stage method obtained are the same.

The two-stage third order L-stable formula with minimization of the principal part of the local truncation error is completely determined (in term of the value of a given in (122)) by the values

$$\begin{aligned} &c_2 = \frac{2}{3}\,, \quad c_3 = 1\,, \quad d_1 = -4\,a\,, \quad d_2 = 6\,a^2\,, \quad d_3 = -4\,a^3\,, \\ &d_4 = a^4\,, \quad n_1 = \frac{1-8\,a}{2}\,, \quad n_2 = \frac{1-12\,a+36\,a^2}{6}\,, \\ &n_3 = \frac{1-16\,a+72\,a^2-96\,a^3}{24}\,, \end{aligned} \tag{123}$$

and making zero all the other parameters.

Now we will describe a three-stage fourth order A-stable method of rational type for separated systems. We begin considering the general form obtained in Section 8, from which we will obtain the formula following the steps:

Step 1. We take the values for the free parameters $a_{4,32}$ and c_3 in (79)

$$a_{4,32} = 0\,, \quad c_3 = \frac{6+\sqrt{6}}{10}\,. \tag{124}$$

Note that the value taken for c_3 is the same that gives us order five with three stages in the scalar case (see [7]).

Step 2. After substituting these values in (79) we substitute the obtained solution (that gives us order four for the three-stage methods of polynomial type) in relations (85–91). We obtain in this manner a family of three-stage methods of rational type and order four, that is completely given in terms of the values of the coefficients d_*.

Step 3. Between all possible choices to obtain a method whose associated linear stability function is given as we want, we take the one obtained by making zero the following coefficients

$$d_{4,3} = d_{4,23} = d_{4,32} = 0\,, \tag{125}$$

and taking the remaining free parameters as follows

$$d_{3,2} = -a\,, \quad d_{4,2} = -3\,a\,, \quad d_{4,22} = 3\,a^2\,, \quad d_{4,222} = -a^3\,, \tag{126}$$

so that only one LU factorization will be necessary per integration step.

Step 4. Finally we get the value of constant a in such a way that the resulting formula becomes A-stable. For this end we obtain a as the root of equation

$-1+12\,a-36\,a^2+24\,a^3=0$ that takes approximately the value

$$a \approx 1.06857902\,, \tag{127}$$

and the linear stability function associated to the method is given in terms of the constant a by

$$R(z) = \frac{6+6(1-3a)z+3(1-6a+6a^2)z^2+(1-9a+18a^2-6a^3)z^3}{6\,(1-a\,z)^3}\,. \tag{128}$$

In [11], pp. 97 we can find this value of a for the A-stability.

The three-stage fourth order A-stable formula is completely determined (in term of the value of a given in (127)) by the values

$$\begin{aligned}
c_2 &= \frac{6-\sqrt{6}}{10}\,, \quad c_3 = \frac{6+\sqrt{6}}{10}\,, \quad c_4 = 1\,, \quad d_{3,2} = -a\,,\\
d_{4,2} &= -3\,a\,, \quad d_{4,3} = 0\,, \quad d_{4,22} = 3\,a^2\,, \quad d_{4,23} = 0\,,\\
d_{4,32} &= 0\,, \quad d_{4,222} = -a^3\,, \quad n_{3,2} = \frac{(6-5\,a)-\sqrt{6}}{5}\,,\\
n_{4,2} &= \frac{1-6\,a}{2}\,, \quad n_{4,3} = \frac{9+\sqrt{6}}{36}\,, \quad n_{4,22} = \frac{18\,a^2-9\,a+1}{6}\,,\\
n_{4,23} &= \frac{6\,(1-9\,a)-(1+6\,a)\sqrt{6}}{72}\,, \quad n_{4,32} = 0\,,\\
n_{4,222} &= \frac{-24\,a^3+36\,a^2-12\,a+1}{24}\,,
\end{aligned} \tag{129}$$

and making zero the remaining parameters.

Finally we will obtain a three-stage fourth order method of rational type for systems being L-stable and minimizing the principal part of the local truncation error. In a previous section we obtained the general form of the three-stage fourth order methods of rational type for systems, that minimize the principal part of the local truncation error. Between many possible choices we give the steps followed by us to obtain the formula:

Step 1. We make zero the free parameter $a_{4,322}$ in (80) and substitute the values obtained in this way in relations (92–104). We get in this manner the coefficients of a family of three-stage fourth order methods of rational type for systems that minimize the principal part of the local truncation error. Any method of this family is completely determined from the values of coefficients d_*.

Step 2. Between all different possibilities we have to obtain a formula whose associated linear stability function is given as we want, we decided to make zero all coefficients d_* that appear multiplied by terms containing the factor S_3.

The remaining free parameters are taken as follows

$$
\begin{aligned}
d_{3,2} = -2\,a\,, \quad d_{3,22} = a^2\,, \quad d_{4,2} = -5\,a\,, \quad d_{4,22} = 10\,a^2\,,\\
d_{4,222} = -10\,a^3\,, \quad d_{4,2222} = 5\,a^4\,, \quad d_{4,22222} = -a^5\,.
\end{aligned}
\tag{130}
$$

In the preceding formula we have introduced coefficient $d_{4,22222}$ which does not appear neither in order four conditions nor in order five conditions (that we take into account to minimize the principal part of the local truncation error). We make this because we look for a L-stable method and so the linear stability function associated to the formula must have a denominator of degree five.

Step 3. Finally we get the value of constant a in such a way that the resulting formula is L-stable. We must take a as the root of polynomial $-1 + 25\,a - 200\,a^2 + 600\,a^3 - 600\,a^4 + 120\,a^5 = 0$ that takes approximately the value

$$
a \approx 0.27805384\,, \tag{131}
$$

and the linear stability function $R(z)$ associated to the resulting method is given in terms of a by

$$
\begin{aligned}
R(z) = & \frac{24+24(1-5a)z+12(1-10a+20a^2)z^2}{24\,(1-a\,z)^5} \\
& + \frac{4(1-15a+60a^2-60a^3)z^3+(1-20a+120a^2-240a^3+120a^4)z^4}{24\,(1-a\,z)^5}\,.
\end{aligned}
\tag{132}
$$

In [11], pp. 98 we can find this value of a giving us the L-stability property.

The obtained coefficients for the method are given by

$$
\begin{aligned}
c_2 = & \frac{6-\sqrt{6}}{10}\,, \quad c_3 = \frac{6+\sqrt{6}}{10}\,, \quad c_4 = 1\,, \quad d_{3,2} = -2\,a\,,\\
d_{3,22} = & a^2\,, \quad d_{4,2} = -5\,a\,, \quad d_{4,22} = 10\,a^2\,, \quad d_{4,222} = -10\,a^3\,,\\
d_{4,2222} = & 5\,a^4\,, \quad d_{4,22222} = -a^5\,, \quad n_{3,2} = \frac{-(3+10\,a)+2\,\sqrt{6}}{5}\,,\\
n_{3,22} = & \frac{(17+60\,a+50\,a^2)-(3+40\,a)\,\sqrt{6}}{50}\,, \quad n_{4,2} = \frac{1-10\,a}{2}\,,\\
n_{4,3} = & \frac{9+\sqrt{6}}{36}\,, \quad n_{4,22} = \frac{60\,a^2-15\,a+1}{6}\,,\\
n_{4,23} = & \frac{6\,(1-15\,a)-(1+10\,a)\,\sqrt{6}}{72}\,, \quad n_{4,32} = \frac{-1+\sqrt{6}}{8}\,,\\
n_{4,33} = & \frac{1+4\,\sqrt{6}}{72}\,, \quad n_{4,222} = \frac{-240\,a^3+120\,a^2-20\,a+1}{24}\,,\\
n_{4,223} = & \frac{3\,(1-20\,a+120\,a^2)+(-1+10\,a+40\,a^2)\,\sqrt{6}}{144}\,,
\end{aligned}
$$

$$n_{4,232} = \frac{3\,(-1+10\,a)+2(1-15\,a)\,\sqrt{6}}{48}\,,$$
$$n_{4,2222} = \frac{600\,a^4-600\,a^3+200\,a^2-25\,a+1}{120}\,, \tag{133}$$

in terms of the value of a given in (131) and making zero the remaining free parameters.

13 Numerical experiments with the two and three-stage A-stable and L-stable methods: Van der Pol's equation.

In order to illustrate the good behaviour of the GRK-methods obtained we will now study some numerical experiments. We will apply our methods to some problems and compare the results obtained with those we get with some classical formulas.

The first problem we consider, involves the well known Van der Pol's equation that is given by

$$\varepsilon\, z'' + (z^2-1)\, z' + z = 0\,, \quad z(0) = a\,, \quad z'(0) = b\,. \tag{134}$$

Note that our methods cannot be applied to the system of first order ODEs given by

$$\begin{aligned} z' &= y & z(0) &= a \\ y' &= \frac{1}{\varepsilon}((1-z^2)\, y - z) & y(0) &= b \end{aligned} \tag{135}$$

we obtain transforming in the usual way this second order equation, because the resulting system is not a separates one. However, using Liénard's coordinates (see [11], pp. 372 for more details) the problem (134) takes the form

$$\begin{aligned} y' &= -z & y(0) &= \varepsilon\, b - a + \frac{a^3}{3} \\ z' &= \frac{1}{\varepsilon}\left(y + z - \frac{z^3}{3}\right) & z(0) &= a \end{aligned} \tag{136}$$

and now our methods can be applied to this system.

We integrate this problem in the interval $[0, 0.5]$, taking $\varepsilon = 10^{-5}$. We have considered the following initial conditions

$$y(0) = 0.66666000001234554549467\,, \qquad z(0) = 2.\,, \tag{137}$$

obtained from those considered in [11], pp. 403, by taking the Liénard's coordinates. With the six methods obtained, we have integrated the preceding problem with fixed stepsize h and we have calculated the relative error obtained in both components at the point 0.5. Errors are measured with respect to a reference solution obtained with a very accurate variable step method (the 'gear' method implemented in MAPLEV, working with 30 digits and taking a tolerance of 10^{-20}) that is enough for our purposes.

For comparison purposes we have also integrated this problem with the two-stage third order Rosenbrock method that can be found for example in [10], pp. 334, and known as Calahan's method.

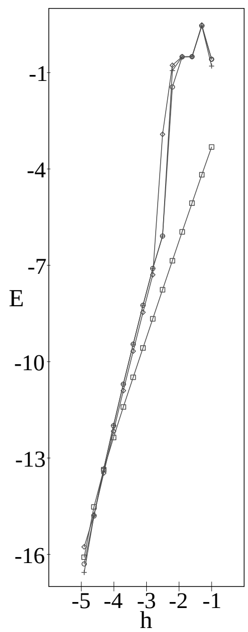

Fig. 7. Relative error (first component) as a function of the stepsize in double logarithmic scale for the third order methods.

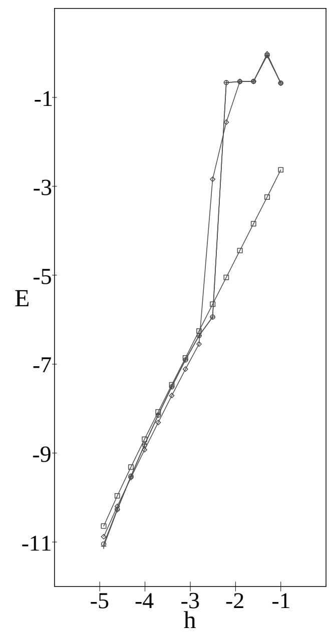

Fig. 8. Relative error (second component) as a function of the stepsize in double logarithmic scale for the third order methods.

In Figures 7 and 8 we show the relative errors corresponding to the first and second components respectively as a function of the stepsize h (taking $h = 0.1 \cdot 2^{-k}$ for $k = 0, 1, 2, \ldots, 12$) in double logarithmic scale for the different third order methods. Calahan's method is represented in these figures by squares. With diamonds we represent the third order A-stable method, with circles the first third order L-stable formula we obtained and with crosses the last third order L-stable method we have developed.

It can be observed in these figures that Calahan's method performs better than our three methods when big values of the stepsize are considered. When we take smaller stepsizes our methods perform very similarly to Calahan's formula and some of them perform even better than this Rosenbrock formula. Note at this point that the problem considered is very stiff, with one of the eigenvalues of the associated Jacobian matrix in the interval $[-300000, -150000]$

and the other eigenvalue being small and negative along the integration interval. Note also that Calahan's method needs an evaluation of the Jacobian matrix associated to the problem per integration step and that our methods, as we have pointed out before, incorporate an approximation to this Jacobian matrix obtained from matrix S_2/h (with no extra evaluations). This explains what happens when the stepsize h is big, because when this is so we have that the approximation that gives matrix S_2 to the Jacobian matrix is usually not too good (and in some problems this gives worse approximations to the solution). It can be expected that this formulas will perform better by using variable stepsizes, but we will not study this here.

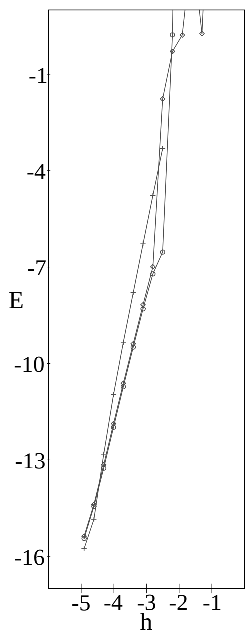

Fig. 9. Relative error (first component) as a function of the stepsize in double logarithmic scale for the fourth order methods.

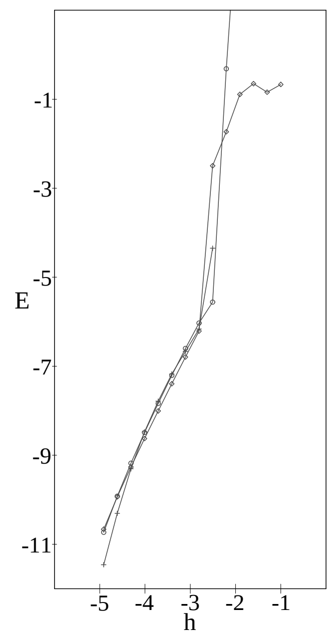

Fig. 10. Relative error (second component) as a function of the stepsize in double logarithmic scale for the fourth order methods.

We repeated the preceding numerical experiment with the three obtained fourth order formulas. Results are shown in Figures 9 and 10 . In this figure we represent with diamonds the A-stable method, with circles the first fourth order L-stable formula obtained and with crosses the last fourth order L-stable method proposed. For the formula represented by crosses in these figures we have eliminated the results that are obtained for great values of the stepsize h. We make this because in some of the integrations the matrix whose inverse we must calculate is singular for any of the integration steps. We also observe that, for big stepsizes, the numerical results are not as good as expected, being worse than those obtained with the third order formulas. The reason for that is the same we have commented previously for the two-stage formulas, but now situation is even worse because the approximation S_3/h to the Jacobian matrix (for big stepsizes) is worse than the obtained from matrix S_2/h. However, it can be observed that reducing the stepsize situation is rapidly much better.

Even though the two and three-stage formulas proposed have some problems for moderate stepsizes (as we have pointed out before) they give good approximations to the exact solution of the problem. In fact, we obtain good approximations to the solution integrating with stepsizes much greater than those we can consider when integrating with any classical explicit formula. The order reduction observed for this problem also occurs for other A-stable and L-stable Runge-Kutta type formulas (see [11], pp. 403–404).

14 Numerical experiments with the two and three-stage A-stable and L-stable methods: Burgers' equation.

Now we will consider another problem. More precisely, we will repeat the numerical experiment of a preceding section with the system of ODEs given by (23). In this problem, obtained by the method of lines approach to the Burgers' equation, we will consider the values $N = 24$ and $\nu = 0.2$.

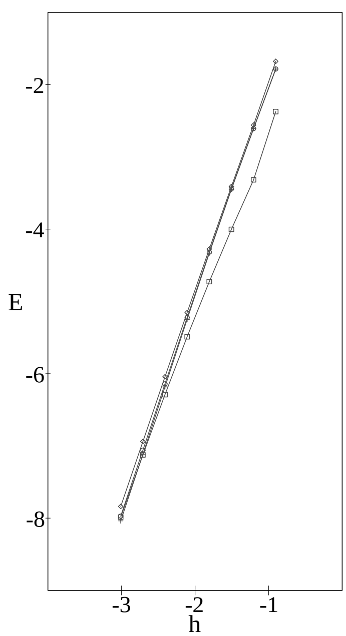

Fig. 11. Error as a function of the stepsize in double logarithmic scale for the third order methods.

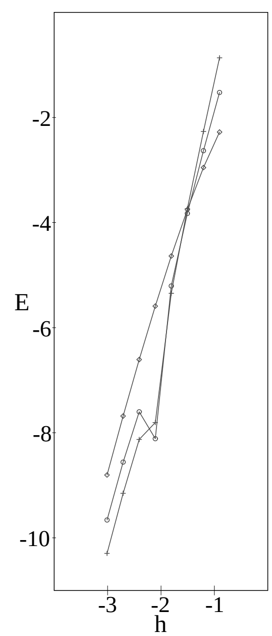

Fig. 12. Error as a function of the stepsize in double logarithmic scale for the fourth order methods.

In Figure 11 we show in double logarithmic scale the error E (measured with the Euclidean norm in $\mathbb{R}^{24}$) at the point $t = 1$, obtained by integrating this problem with the different third order methods, taking fixed stepsize $h = 2^{-k}$ for the values $k = 3, 4, \ldots, 10$. We have represented the methods in this figure with the same symbols as in Figures 7 and 8. It can be observed in the figure that Calahan's method performs slightly better than our proposed formulas when big values of the stepsize h are considered, but when this stepsize is reduced our methods perform very similarly to Calahan's formula and some of them perform even better than the Calahan's formula. For this problem the three proposed formulas give very similar approximations to solution, as can be seen in the figure. It is easily seen that the slopes of the curves represented in the figure are near to three (as expected).

When we repeat the last numerical experiment taking the three fourth order methods, we get Figure 12. We have represented the formulas in this figure with the same symbols as in Figures 9 and 10. It can be observed that, for big values of the stepsize, the approximations we get from the the fourth order methods are in some cases slightly worse than those obtained from the third order methods. However, for smaller stepsizes the fourth order methods perform much better than the third order ones. We also observe that the method that gives the better approximations for small stepsizes is that represented by crosses in the figure (but this is also the method with the greatest computational cost associated). The slopes of the curves represented in the figure are nearly four when the stepsize considered is reduced.

15 Conclusions.

In this second part we have introduced and studied a new family of methods for the numerical integration of some systems of ODEs. These new methods seem quite promising, for instance in the context of solving some nonlinear parabolic equations (by the method of lines approach). We have shown that with the family of linearly implicit methods we have proposed here, it is possible to attain order three with only two stages and order four with three stages, as well as some interesting linear stability properties such as A-stability and L-stability. Our methods do not require Jacobian evaluations in their implementation and therefore require less computational work than other classical implicit and linearly implicit methods that can be applied to stiff problems.

In subsequent works we will study as in [2] how to obtain formulas (belonging to the family of GRK-methods) from any prefixed linear stability function. This can be of great interest when considering perturbed problems for which the exact solution of the unperturbed problem is known in advantage, because we can obtain methods specifically designed to integrate exactly the unperturbed problem.

We will also extend our GRK-methods in order to obtain formulas with built-in error estimates, that is, embedded GRK-methods.

References

[1] R. Alexander, Diagonally implicit Runge-Kutta methods for stiff O.D.E.'s, *SIAM J. Numer. Anal.* **14** (1977) 1006–1021.

[2] J. Álvarez, Obtaining New Explicit Two-Stage Methods for the Scalar Autonomous IVP with Prefixed Stability Functions, *Intl. Journal of Applied Sc. & Computations* **6** (1999) 39–44.

[3] J. Álvarez, *Métodos GRK para ecuaciones diferenciales ordinarias*, Universidad de Valladolid, Spain, Dpto. de Matemática Aplicada a la Ingeniería, Tesis - Ph.D. Thesis, 2002, 149 pp.

[4] J. Álvarez and J. Rojo, New A-stable explicit two-stage methods of order three for the scalar autonomous IVP, in: P. de Oliveira, F. Oliveira, F. Patrício, J.A. Ferreira, A. Araújo, eds., *Proc. of the 2nd. Meeting on Numerical Methods for Differential Equations, NMDE'98* (Coimbra, Portugal, 1998) 57–66.

[5] J. Álvarez and J. Rojo, A New Family of Explicit Two-Stage Methods of order Three for the Scalar Autonomous IVP, *Intl. Journal of Applied Sc. & Computations* **5** (1999) 246–251.

[6] J. Álvarez and J. Rojo, Special methods for the numerical integration of some ODE's systems, *Nonlinear Analysis: Theory, Methods and Applications*, **47** (2001) 5703–5708.

[7] J. Álvarez and J. Rojo, An improved class of generalized Runge-Kutta methods for stiff problems, Part I: The scalar case. *Applied Mathematics and Computations* **130** (2002) 537–560.

[8] J. Álvarez and J. Rojo, An improved class of generalized Runge-Kutta-Nyström methods for special second order differential equations, in *Proc. of the International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE 2002* (Alicante, Spain, 2002) **I** 11–20. (Alicante, Spain).

[9] J.C. Butcher, Implicit Runge-Kutta processes, *Math. Comp.* **18** (1964) 50–64.

[10] J.C. Butcher, *The Numerical Analysis of Ordinary Differential Equations: Runge-Kutta and General Linear Methods* (Wiley, Chichester, 1987).

[11] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems* (Springer-Verlag, Berlin, 1996).

[12] P. Kaps, Rosenbrock-type methods, in: G. Dahlquist and R. Jeltsch, eds., *Numerical methods for solving stiff initial value problems, Proceedings, Oberwolfach 28/6–4/7 1981*, Bericht Nr. 9, Inst. für Geometrie und Praktische Mathematik der RWTH Aachen (Aachen, Germany, 1981) 5 pp.

[13] P. Kaps, S. W. H. Poon and T. D. Bui, Rosenbrock Methods for Stiff ODEs: A Comparison of Richardson Extrapolation and Embedding Technique, *Computing* **34** (1985) 17–40.

[14] P. Kaps and P. Rentrop, Generalized Runge-Kutta Methods of Order Four with Stepsize Control for Stiff Ordinary Differential Equations, *Numer. Math.* **33** (1979) 55–68.

[15] P. Kaps and G. Wanner, A Study of Rosenbrock-Type Methods of High Order, *Numer. Math.* **38** (1981) 279–298.

[16] J.D. Lambert, *Numerical Methods for Ordinary Differential Systems. The Initial Value Problem* (Wiley, Chichester, 1991).

[17] S.P. Nørsett and A. Wolfbrandt, Order Conditions for Rosenbrock Type Methods, *Numer. Math.* **32** (1979) 1–15.

[18] A. Prothero and A. Robinson, On the stability and accuracy of one-step methods for solving stiff systems of ordinary differential equations, *Math. Comput.* **28** (1974) 145–162.

[19] H.H. Rosenbrock, Some general implicit processes for the numerical solution of differential equations, *Comput. J.* **5** (1963) 329–330.

[20] J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems* (Chapman-Hall, London, 1993).

[21] S. Scholz, Order Barriers for the B-Convergence of ROW Methods, *Computing* **41** (1989) 219–235.

[22] T. Steihaug and A. Wolfbrandt, An Attempt to Avoid Exact Jacobian and Nonlinear Equations in the Numerical Solution of Stiff Differential Equations, *Math. Comp.* **33** (1979) 521–534.

[23] J. G. Verwer, *S*-Stability Properties for Generalized Runge-Kutta Methods, *Numer. Math.* **27** (1977) 359–370.

[24] H. Zedan, Avoiding the exactness of the Jacobian matrix in Rosenbrock formulae, *Comput. Math. Appl.* **19** (1990) 83–89.