NEW IMPLICIT MULTISTEP METHOD FOR ODE's

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Abstract

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A new class of multistep methods for stiff ordinary differential equations is presented. The method is based on the transformation of the arguments of the original system into purely algebraic combinations of the solutions of previous steps. The scheme differs from the classical multistep methods in that the state variables, instead of functions of them, are aproximated by means of linear combination of previous steps. A family of coefficients is deduced from a combined analysis of convergence order and stability. Numerical results are presented for three test problems.

Key words: multistep methods, ordinary differential equations, A-stability, convergence order.

Resumen

Se presenta una nueva clase de método multipaso para ecuaciones diferenciales ordinarias con stiff. El método se basa en la transformación de los argumentos del sistema original en un sistema puramente algebraico utilizando las soluciones de los pasos anteriores. El esquema difiere de los clásicos métodos multipaso en que las variables de estado son reemplazadas por funciones, las cuales son aproximadas por medio de una combinación lineal de las soluciones previas. Una familia de coeficientes se deduce a partir de un análisis combinado de orden de convergencia y estabilidad. Por último se presentan resultados numéricos para tres problemas test.

Palabras clave: métodos multipaso, ecuaciones diferenciales ordinarias, A-estabilidad, orden de convergencia.

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1. Introduction

The use of implicit numerical methods is convenient when solving general stiff Ordinary Differential Equations (ODE) problems. Their use, in turn, requires the solution of a corresponding discrete problem, which is one of the main concerns in the actual implementation of the methods. Linear implicit multistep methods and, in particular, Backward Differentiation Formulae (BDF) [6] [2] are regularly used for the numerical solution of stiff initial value problems. In turn, implicit methods require solving at each integration step an algebraic problem, whose dimension is a multiple of the corresponding continuous one [3].

A high-quality numerical method to solve stiff ODE should have good accuracy and some wide region of absolute stability ([5], [8], [9] and [10]). The latter imposes a strong limitation on the choice of suitable methods for stiff problems.

In the present paper a new class of implicit multistep method is derived, having good stability and convergence properties compared with equivalent linear schemes. The difference with classical multistep methods is the transformation of the differential system into a purely algebraic system by introducing estimation functions not only for the derivatives but also for the state variables. In this sense, the methodology used in the current method can be understood as a variant of the basic theory of classical multistep methods. In the last section, numerical experiments are presented comparing the new method with BDF.

2. Linear Multistep Method

Let us consider the initial value problem (IVP) [7]

$$y^{(1)}(t) = f(y), y(t_0) = y_0 \tag{1}$$

where $t \in [t_0, t_0 + Nh]$ (N being a natural number and h a constant time step), $y : [t_0, t_0 + Nh] \to \mathrm{R}^m$, $y^{(1)}$ stands for the first temporal derivative, and $f : \mathrm{R}^m \to \mathrm{R}^m$ is continuous and differentiable.

The classical linear multistep method can be written in the general form [2]

$$\sum_{i=0}^{k} \alpha_i y_{n-i} = h \sum_{i=0}^{k} \beta_i f\left(y_{n-i}\right) , \tag{2}$$

where $\alpha_i,\ \beta_i$ are parameters to be determined and $y_n = y(t_0 + nh)$. The method is *explicit* if $\beta_0 = 0$ and *implicit* otherwise. A multistep method is of order p if and only if [3]:

$$\sum_{i=0}^{k} \alpha_i i^q = q \sum_{i=0}^{k} \beta_i i^{q-1} + \mathrm{O}\left(h^p\right), \tag{3}$$

with $0 \leq q \leq p$. The well-known multistep scheme BDF is given by

$$\sum_{i=0}^{k} \alpha_i y_{n-i} = h\beta_0 f\left(y_n\right). \tag{4}$$

This scheme is a class of k-step formula of order k, and for $k = 2$, the BDF coefficients are [2]

$$\alpha_0 = \frac{3}{2},\ \alpha_1 = -2,\ \alpha_2 = \frac{1}{2},\ \beta_0 = 1. \tag{5}$$

3. New multistep transformation

The general multistep formula (*i.e.* Eq. 2) is essentially a transformation of the differential Eq. 1 into a purely algebraic equation by means of the estimators:

$$y^{(1)} \to \frac{1}{h} \sum_{i=0}^{k} \alpha_i\, y_{n-i}\ ,\ f\left(y\right) \to \sum_{i=0}^{k} \beta_i\, f\left(y_{n-i}\right). \tag{6}$$

Let us propose the following alternative set of transformations:

$$y \to \sum_{i=0}^{k} A_i\, y_{n-i}\ ,\ y^{(1)} \to \frac{1}{h} \sum_{i=0}^{k} B_i\, y_{n-i}. \tag{7}$$

where A_i and B_i are coefficients satisfying $\sum_{i=0}^{k} B_i = 0$ and $\sum_{i=0}^{k} A_i = 1$. Eq. 7 lead to the following alternative multistep algebraic equation:

$$\frac{1}{h} \sum_{i=0}^{k} B_i y_{n-i} = f\left(\sum_{i=0}^{k} A_i y_{n-i}\right). \tag{8}$$

To make clear the deduction of the coefficients, let us consider a two-step instance of Eq. 8 ($k = 2$). The general method to determine the coefficients A_i and B_i, can be generalized from this particular case.

3.1. Convergence order.

Expanding y_{n-2} and y_n in Taylor series around (t-h) leads to:

$$\begin{aligned} y_n &= y_{n-1}^{(0)} + h\, y_{n-1}^{(1)} + \tfrac{h^2}{2} y_{n-1}^{(2)} + \mathrm{O}\left(h^3\right), \\ y_{n-2} &= y_{n-1}^{(0)} - h\, y_{n-1}^{(1)} + \tfrac{h^2}{2} y_{n-1}^{(2)} + \mathrm{O}\left(h^3\right), \end{aligned} \tag{9}$$

where $y_n^{(k)}$ stands for the k-th derivative of y respect to time. Combining Eqs. 7 and 9 yields:

$$\begin{array}{l} y_n^{(1)} = (B_0 - B_2)\, y_{n-1}^{(1)} + \\ (B_0 + B_2)\, \frac{h}{2} y_{n-1}^{(2)} + \mathrm{O}\left(h^2\right), \\ y_n = y_{n-1}^{(0)} + (A_0 - A_2)\, h y_{n-1}^{(1)} + \mathrm{O}\left(h^2\right). \end{array} \quad (10)$$

Expanding now f_j around $(t\text{-}h)$, gives

$$f\left(y_n\right) = f\left(y_{n-1}\right) + \nabla^T f\left(y_{n-1}\right)\ y_{n-1}^{(1)}\ h + \mathrm{O}\left(h^2\right), \quad (11)$$

where $\nabla^T f\left(y_n\right)$ stand for the transpose gradient of $f(y)$ (taken separately to each component f_j evaluated at $y = y_n$.

Likewise, expanding the right term of the Eq. 8, gives:

$$\begin{array}{l} f\left(\sum_{i=0}^{2} A_i y_{n-i}\right) = f^{(0)}\left(y_{n-1}\right) + \\ (A_0 - A_2)\ \nabla^T f\left(y_{n-1}\right)\ y_{n-1}^{(1)}\ h + \mathrm{O}\left(h^2\right). \end{array} \quad (12)$$

The relation between $f\left(y_n\right)$ and $\nabla^T f\left(y_n\right)$ with $y_n^{(k)}$ can be found by successive differentiations of Eq. 1. Combining Eq. 10 to Eq. 12 yields:

$$\begin{array}{l} (B_0 - B_2)\, y_{n-1}^{(1)} = f\left(y_{n-1}\right), \\ (B_0 + B_2)\, y_{n-1}^{(2)} \frac{h}{2} = (A_0 - A_2)\ \nabla^T f\left(y_{n-1}\right)\ y_{n-1}^{(1)} h, \end{array} \quad (13)$$

which leads to the following set of algebraic equations for the coefficients A_i and B_i:

$$\begin{array}{l} \sum_{i=0}^{2} A_i = 1, \\ \sum_{i=0}^{2} B_i = 0, \\ (B_0 - B_2 - 1)\, f\left(y_{n-1}\right) = 0, \\ (B_0 + B_2 - 2A_0 + 2A_2)\ \nabla^T f\left(y_{n-1}\right)\ f\left(y_{n-1}\right) = 0. \end{array} \quad (14)$$

Eqs. 14 is a set of 4 algebraic equations with 6 unknowns. Therefore, there is a family of coefficients A_i and B_i that ensures $\mathrm{O}\left(h^2\right)$ convergence; that is:

$$\begin{array}{l} A_0 = \frac{1}{2} - \frac{B_1}{4} - \frac{A_1}{2},\ \ A_2 = \frac{1}{2} + \frac{B_1}{4} - \frac{A_1}{2}, \\ B_0 = \frac{1}{2} - \frac{B_1}{2},\ \ B_2 = -\frac{1}{2} - \frac{B_1}{2}. \end{array} \quad (15)$$

3.2. 0-Stability. As the name implies, 0-stability is concerned whit what happens in the limit $h \to 0$ [2]. The linear multistep method is 0-stable if all k roots ξ_i of the characteristic polynomial:

$$\rho\left(\xi\right) = \sum_{i=0}^{2} B_i \xi^{2-i} = 0, \quad (16)$$

satisfy $|\xi_i| \leq 1$. If the root condition is satisfied, the method is accurate to order p. Therefore provided that the initial values are accurate to order p, the method is convergent to order p.

Lemma 1. *If $B_1 \leq 0$, then the roots ξ_1 and ξ_2 of $\rho\left(\xi\right)$ verify that $|\xi_i| \leq 1$, for $i = 1, 2$.*

Proof. Applying Eq. 15 to Eq. 16 yields

$$\rho\left(\xi\right) = \xi^2 \left(\frac{1}{2} - \frac{B_1}{2}\right) + \xi\, B_1\ - \frac{1}{2} - \frac{B_1}{2} = 0. \quad (17)$$

Then, the roots are

$$\xi_{1,2} = \frac{-B_1 \pm 1}{1 - B_1}. \quad (18)$$

Next, it can be observed that

$$|\xi_1| = \left|\frac{-B_1 + 1}{1 - B_1}\right| = 1, \quad (19)$$

and

$$|\xi_2| = \left|\frac{-B_1 - 1}{1 - B_1}\right| = \left|-1 - \frac{2B_1}{1 - B_1}\right| \leq 1, \quad (20)$$

for $B_1 \leq 0$.

3.3. A-Stability. The stability of the linear multistep method is given by the stability of the resulting difference equation [2]. Applying Eq. 8 for k=2 to the linear test equation $y = \lambda y$, ($\lambda \in$C), yields:

$$\sum_{i=0}^{2} \left(B_i - \lambda A_i\right) y_{n-i} = 0. \quad (21)$$

The stability of Eq. 21 is demonstrated by ensuring the stability of the difference equation. The difference equation is stable if all roots ξ_i of:

$$\phi\left(\xi\right) = \sum_{i=0}^{2} \left(B_i - A_i h\lambda\right) \xi^{2-i} = 0, \quad (22)$$

satisfy $|\xi_i| \leq 1$.

When f is linear and k=2, a necessary condition for A-stability is given by [2] $Re\left(z\right) \geq 0$, where

$$z = \frac{\sum_{i=0}^{2} B_i q^{2-i}}{\sum_{i=0}^{2} A_i q^{2-i}}, \quad (23)$$

for all (unitary) complex numbers $q = \cos\theta + i \sin\theta$, for $\theta \in [0, 2\pi]$.

Figures 1 and 2 compare the absolute stability regions for the proposed method and the BDF method for different sets of coefficients. However, numerical computations show that, in the general case, those conditions are not sufficient. For example, for the values $A_1 \geq 1/2$ and $B_1 \leq 0$ the method is A-unstable.

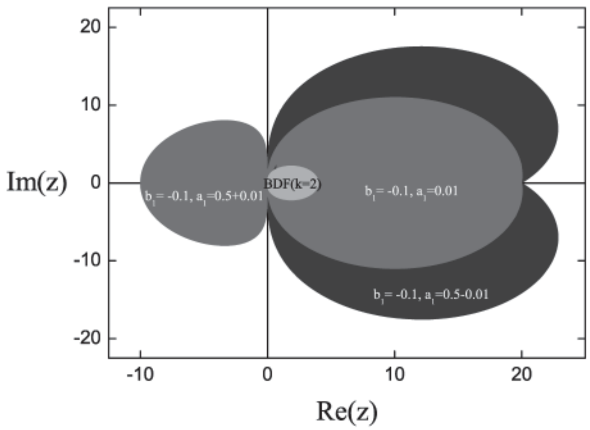

Figure 1. Absolute stability region of the present method and the BDF method

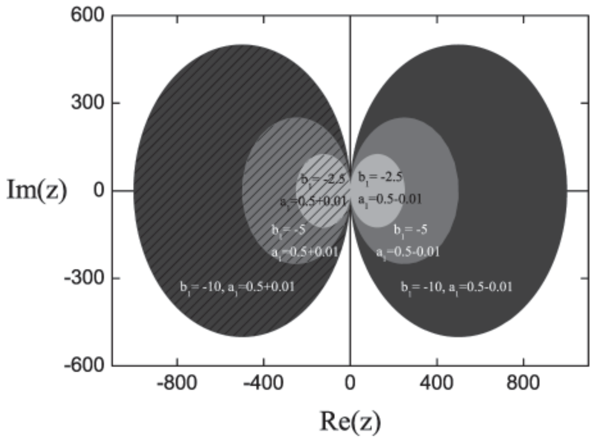

Figure 2. Absolute stability region of the present method and the BDF method

For the particular case of k=2 a range for the coefficients that make our method A-stable can be found. We resume this result in the next lemma.

Lemma 2. *If* $B_1 \leq 0$, $A_1 < 1/2$ *and* $Re(z) < 0$, *then all the roots* ξ *of the* $\phi(\xi)$ *verify* $|\xi| \leq 1$.

Proof. Applying into 15 and 16, the roots of the difference equation are:

$$\xi_{1,2}(z) = \frac{A_1\, z - B_1 \pm \sqrt{1 - \left(B_1 - \frac{B_1^2}{2}\right) z - \left(1 - 2A_1 - \frac{B_1^2}{2}\right) z^2}}{1 - B_1 - \left(1 - A_1 - \frac{B_1}{2}\right) z}. \tag{24}$$

The aim is to study the function $\xi_{1,2}(z)$ of the complex variable z, for the values of A_1, B_1 and z defined in the hypothesis. First, observe that the denominator of Eq. 24 vanishes for

$$z = \frac{2B_1 - 2}{2A_1 - 2 + B_1}, \tag{25}$$

which is a real positive number, meaning that it will never occur as $Re(z) < 0$. Then $\xi_{1,2}(z)$ is an analytic function in C_- and hence, by the *Principle of Maximum* [4], for every open and convex set $\Omega \subset C_-$, the maximum of $|\xi_{1,2}(z)|$ in Ω is obtained at the boundary. So, it is sufficient to prove that the following limit inequalities are verified:

$$\begin{aligned} &\lim_{u \to -\infty} |\xi_{1,2}(u + iv)| \leq 1, \ \forall v \in R\,, \\ &\lim_{u \to \pm\infty} |\xi_{1,2}(u + iv)| \leq 1, \ \forall v \in R_- \bigcup \{0\}\,. \end{aligned} \tag{26}$$

Which are easily verified for $B_1 \leq 0$, $A_1 < 1/2$ and $Re(\lambda) < 0$, as require the lemma, *q.e.d.*

Remark. Although the proposed scheme is A-stable for $B_1 \leq 0$ and $A_1 < 1/2$, the numerical solution of the resulting algebraic system is compromised when the absolute values of these coefficients become too large. Heuristic tests have shown that efficient numerical schemes can be ensured keeping a lower bound of -5 for both coefficients.

4. Numerical experiments

In order to assess its performance the new multistep method was applied to the integration of specific equations using $B_1 = -1{,}5$ and $A_1 = 0{,}1$. This method was compared with the BDF and Adams-Bashforth-Moulton methods for k=2.

4.1. Ricatti equation (m = 1).

Let us consider the following Ricatti equation [1]

$$y^{(1)} = -2 - y + y^2, \tag{27}$$

with initial value $y_0 = 1{,}8$. The exact solution is given by:

$$y(t) = 2 - \frac{3}{1 + 14e^{-3t}}, \tag{28}$$

Figure 3 shows the absolute difference between the analytic and the numerical solutions for $h = 0.01$. It can be observed that the numerical solutions obtained by all methods are similar; and these are always below the order $O\left(h^2\right)$.

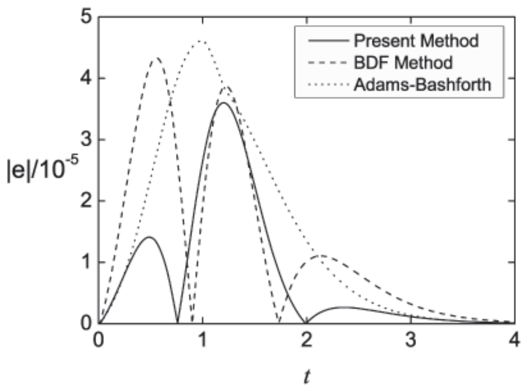

Figure 3. Absolute difference $|e|$ between the analytic and the numerical solutions ($h = 0{,}01$)

4.2. Stiff linear case.

An example of a stiff linear equation is:

$$y^{(3)} = -\left(1003y^{(2)} + 3002y^{(1)} + 2000y\right), \qquad (29)$$

with initial value $y_0 = 1$, $y_0^{(1)} = -1{,}5$ and $y_0^{(2)} = 2{,}5$. The exact solution is given by:

$$y(t) = 0{,}5\left(e^{-t} + e^{-2t}\right). \qquad (30)$$

The stiffness ratio, given by [2]

$$R = \frac{\max\limits_{1\le i\le n} |Re\left(\lambda_i\right)|}{\min\limits_{1\le i\le n} |Re\left(\lambda_i\right)|}, \qquad (31)$$

where λ_i are the eigenvalues of the Jacobian matrix, results R = 1000. This indicates that the stiffness of the system is very high.

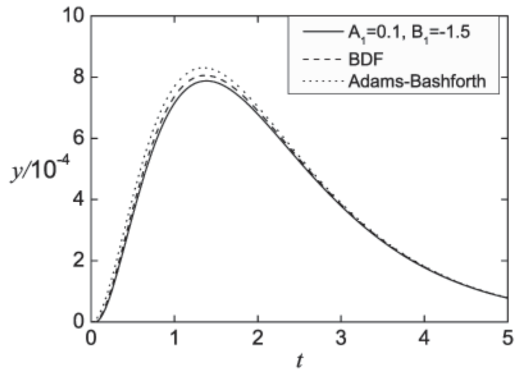

Figure 4. Absolute difference $|e|$ between the analytic and the numerical solutions ($h = 0{,}01$)

Figure 4 shows the temporal evolution of the absolute difference $|e|$ between the analytic and the numerical solutions for y ($h = 0.01$). It can be seen that the three methods give very similar results, whose departure from the exact solution are always below the order of convergence.

4.3. Elastic pendulum.

The elastic pendulum (figure 5) is represented by a fourth-order no-linear system whose natural variables are the string length, r, the inclination angle with respect to the vertical, θ, and their respective temporal derivatives, z and w, that is [11]:

$$\begin{aligned} r^{(1)} &= z, \\ \theta^{(1)} &= w, \\ z^{(1)} &= rw^2 - \tfrac{k}{m}\left(r - L\right) + g\cos\theta, \\ w^{(1)} &= \left(-g\sin\theta - 2zw\right)\tfrac{1}{r}. \end{aligned} \qquad (32)$$

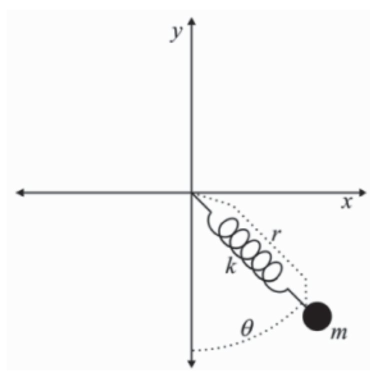

Figure 5. Elastic Pendulum

Comparisons were made using the following parameters and initial conditions: $k = 7$, $L = 1$, $m = 0{,}1$, $g = 9{,}8$,

$r_0 = 1$, $\theta_0 = \frac{\pi}{2}$, $r_0 = 0$ and $\theta_0 = 0$. Figure 6 shows the trajectory of the mass in the (x, y) plane. Figure 7 shows that the stiffness ratio is always much greater than 1, which indicates that the stiffness of the system is high. Figures 8 and 9 shows the absolute differences, $|e_r|$ and $|e_\theta|$, for the variables r and θ calculated between the present method ($B_1 = -1{,}5$ and $A_1 = 0{,}1$) compared BDF ($B_1 = -2$ and $A_1 = 0$) and Adams-Bashforth-Moulton method, showing good agreement.

It can be seen that the differences do not escalate, remaining bounded even for very long times.

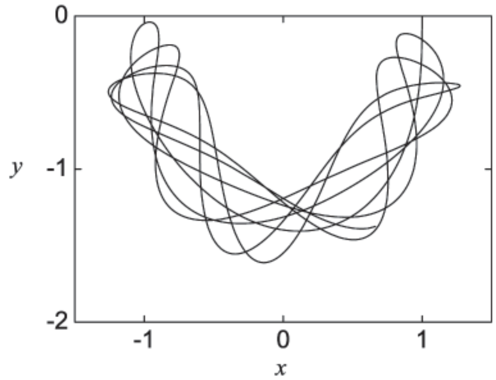

Figure 6. Trajectory of the mass tied to an elastic pendulum in the (x, y) plane

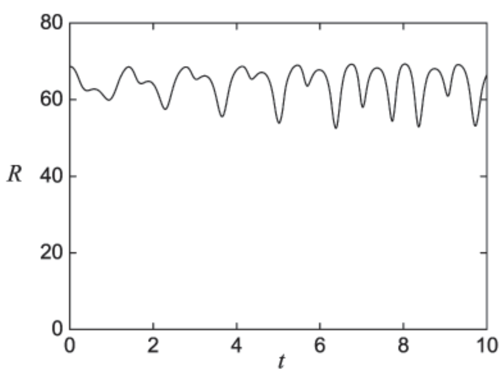

Figure 7. Temporal evolution of the stiffness ratio R of the elastic pendulum

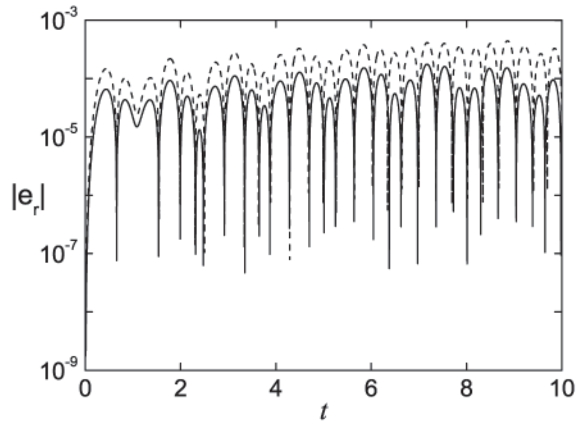

Figure 8. Absolute difference $|e_r|$ of the variable r calculated with present method ($B_1 = -1{,}5, A_1 = 0{,}1$) and (solid) BDF ($B_1 = -2, A_1 = 0$), (dashed) Adams-Bashforth-Moulton method. The time step is $h = 0{,}01$

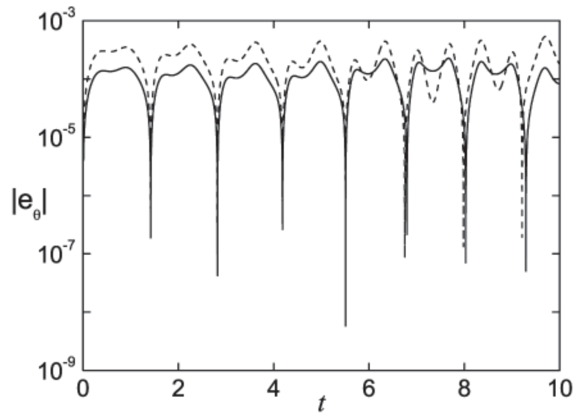

Figure 9. Absolute difference $|e\theta|$ of the variable θ calculated with present method ($B_1 = -1{,}5, A_1 = 0{,}1$) and (solid) BDF ($B_1 = -2, A_1 = 0$), (dashed) Adams-Bashforth-Moulton method. The time step is $h = 0{,}01$

Table 1 shows the ratio between the CPU time divided by the simulated time, for each method, with respect to the time step h. As expected, the time ratio decreases as h increases, being the present method better than the Adams-Bashforth-Moulton one.

Tabla 1. Ratios between CPU time and simulated time ($B_1 = -1{,}5, A_1 = 0{,}1$).

h	Adams-Bashforth-Moulton	BDF	Present method
10-4	0.186	0.184	0.182
10-3	0.025	0.023	0.022
10-2	0.002	0.001	0.001

5. Conclusions

A class of second order multistep methods that produce good candidates for the solution of stiff problems was presented. The class includes as a special case the BDF method. The scheme differs from the classical multistep methods in that the state variables, instead of the functions of them, are approximated by means of linear combination of previous steps. This feature can be usefulness in the design of object-oriented numerical solvers, since the state variables are natural candidates for object definitions.

For a suitable choice of the parameters, the scheme was proved to be A-stable using the Maximum Principle of the theory of complex functions. With several numerical examples it has been also shown that the computation time is approximately the same as the BDF and Adams-Bashforth-Moulton methods, providing a larger stability region. Moreover, the results presented here open the possibility of extending the methodology to DAE systems, since its generalization is straightforward.

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