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NEW A-STABLE NUMERICAL METHOD FOR DIFFERENTIAL EQUATIONS

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Abstract. Stiff problems cause singular computational difficulties because explicit methods cannot solve these problems without rigorous limitations on the step size. To obtain high order A-stable methods, it is traditional to turn to Runge-Kutta methods or to linear multistep methods. A new multistep method is proposed for differential-algebraic equations, based in the application of estimation functions for the derivatives and the state variables, which permits the transformation of the original system into a linear algebraic system with non-linear corrections, using the solutions of the previous steps. The originality introduced is a formula for the estimation function coefficients, which is deduced from a combined analysis of stability and convergence order. Numerical experiments are presented comparing the new method with other classical methods.

1 INTRODUCTION

In general, a system of ordinary differential equations (ODEs) can be expressed in the normal form

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

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

The derivatives of the dependent variables y are expressed explicitly in terms of the independent variable, t, and the dependent variables, y. As long as the function f has sufficient continuity, a unique solution can always be found for an initial value problem where the values of the dependent variables are given at a specific value of the independent variable.

The last three decades mathematical modeling involves problems that are modeled as systems of implicit differential-algebraic equations (DAEs). Such systems arise in designing electric circuits (microchips for computers), mechanics (kinematics equations), nuclear reactor safety analysis, and others (Hairer and Wanner 1996). The general form of a system of DAEs is

$$F\left(t, y, y^{(1)}\right) = 0\ ,\ y(t_0) = y_0\ ,\ y^{(1)}(t_0) = y_0^{(1)}\ , \tag{2}$$

where the Jacobian with respect to $y^{(1)}$ may be singular.

In DAEs the derivatives are not generally expressed explicitly and typically derivatives of some of the dependent variables do not appear in the equations. A system of DAEs can be converted to a system of ODEs by differentiating it with respect to the independent variable t. The *index* of a DAE is effectively the number of times you need to differentiate the DAEs to get a system of ODEs (Ascher and Petzold 1998). Even though the differentiation is possible, it is not generally used as a computational technique because some of the properties of the original DAEs are often lost in numerical simulations of the differentiated equations.

Recently, a new class of multistep methods (HMM) was developed for ODEs stiff (Boroni 2007). The method is based in the application of estimation functions not only of the derivatives but also of the state variables, which leads to the transformation of the original system in a purely algebraic system using the solutions of previous steps. An adaptive formula for the estimation function coefficients is produced, allowing it to be A-stable, with convergence order O(h^3). In this paper the extension of the HMM for index-1 DAE is presented. The method is applied to the original system DAE without converting it to ODE, and the results of numerical experiments are presented.

2 HYBRID MULTISTEP METHOD (HMM) APPLIED TO ODE STIFF

The general multistep method can be written in the form (Ascher and Petzold 1998)

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = h \sum_{j=0}^{k} \beta_j f_{n-j} \,, \tag{3}$$

where α_j, β_j are parameters to be determined, $f_n = f(y_n)$, and $y_n = y(t_0 + nh)$, being h a constant time step.

A order of a multistep method is p if and only if (Butcher 2003)

$$\sum_{j=0}^{k} \alpha_j j^q = q \sum_{j=0}^{k} \beta_j j^{q-1} + \mathrm{O}(h^p), \tag{4}$$

with $0 \le q \le p$.

A popular multistep scheme, which will be used later in this article for comparison, is the Backward Differentiation Formula (BDF) (Gear 1971, Ascher and Petzold 1998), which is given by

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = h \beta_0 f_n \,. \tag{5}$$

This scheme is a class of k-step formulas of order k. Their distinguishing feature is that f is evaluated only at the current step, (t_n, y_n).

The general multistep formula (Eq. 3) is basically a transformation of Eq. 1 (differential) into a purely algebraic equation by means of the estimators

$$\begin{aligned} y_n^{(1)} &\to \frac{1}{h} \sum_{i=0}^{k} \alpha_i y_{n-i} \,, \\ f(y_n) &\to \sum_{i=0}^{k} \beta_i f(y_{n-i}). \end{aligned} \tag{6}$$

The HMM method applied to ODE propose the following alternative set of transformations for $y_j, y_j^{(1)} : 1 \le j \le m$

$$\begin{aligned} y_{n,j} &\to \sum_{i=0}^{k} A_{i,j} y_{n-i,j}, \\ y_{n,j}^{(1)} &\to \frac{1}{h}\sum_{i=0}^{l} B_{i,j} y_{n-i,j}, \end{aligned} \tag{7}$$

where $A_{i,j}$ and $B_{i,j}$ are coefficients satisfying $\sum_{i=0}^{l} B_{i,j} = 0$ and $\sum_{i=0}^{k} A_{i,j} = 1$. Eqs. 3 and 7 lead to the following alternative multistep algebraic equation

$$\frac{1}{h}\sum_{i=0}^{k} B_{i,j} y_{n-i,j} = f_j \begin{pmatrix} \sum_{i=0}^{l} A_{i,0} y_{n-i,1} \\ \dots \\ \sum_{i=0}^{l} A_{i,m} y_{n-i,m} \end{pmatrix}. \tag{8}$$

Letting $k = l = 2$ (the general method to determine the coefficients $A_{i,j}$ and $B_{i,j}$, can be easily deduced from this particular case.), Eqs. 7 and 8 become

$$\begin{aligned} y_j &\to \sum_{i=0}^{2} A_{i,j} y_{n-i,j}, \\ y_j^{(1)} &\to \frac{1}{h}\sum_{i=0}^{2} B_{i,j} y_{n-i,j}, \\ \frac{1}{h}\sum_{i=0}^{2} B_{i,j} y_{n-i,j} &= f_j \begin{pmatrix} \sum_{i=0}^{2} A_{i,0} y_{n-i,0} \\ \dots \\ \sum_{i=0}^{2} A_{i,m} y_{n-i,m} \end{pmatrix}. \end{aligned} \tag{9}$$

Therefore, there is a family of coefficients $A_{i,j}$ and $B_{i,j}$ that ensures $O(h^3)$ convergence

$$\begin{aligned} A_{0,j} &= \frac{1}{6} - \frac{B_{1,j}}{4} + c_j, \; A_{1,j} = \frac{2}{3} - 2c_j, \\ A_{2,j} &= \frac{1}{6} + \frac{B_{1,j}}{4} + c_j, \; B_{0,j} = \frac{1}{2} - \frac{B_{1,j}}{2}, \\ B_{2,j} &= -\frac{1}{2} - \frac{B_{1,j}}{2}, \; c_j = \frac{\left(f^T H_{f_j} f\right)\left(4 - 3B_{1,j}\right)}{24\left(\nabla^T f_j \, J_f^T f\right)}. \end{aligned} \tag{10}$$

In Eqs. 10, f, H_{f_j} and ∇f are evaluated at y_{n-1}. Hence, every term c_j can be seen as a non-linear correction applied in every step to the estimator coefficients of y_j in order to increase the convergence order of the scheme. Eqs. 10 show that all the coefficients $B_{i,j}$ are the same for all variables (*i.e.* independent of j), whereas the coefficients $A_{i,j}$ are different for each variable through c_j. In the particular case that f is linear (*i.e.* $H_j = 0$), $c_j = 0$, and all coefficients $A_{i,j}$ are the same for all variables y_j.

In order to produce a robust method for stiff problems the property A-stability of the method should be ensured. A method is A-stable if, applied to a stable linear set of differential equations, the resulting iterative scheme is also stable independently of h (Ascher and Petzold 1998). In that way, ensuring A-stability, h is determined just for precision purposes, without restrictions on linear stability. Such methods are considered good candidates to solve stiff problems.

Following (Ascher and Petzold 1998) the A-stability, which means that the finite difference solution corresponding to a decreasing exact solution is also decreasing for every value of h, is given by

$$\mathrm{Re}(z) \geq 0 , \tag{11}$$

where

$$z = \frac{\sum_{i=0}^{2} B_i q^{2-i}}{\sum_{i=0}^{2} A_i q^{2-i}} , \tag{12}$$

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

That is, the scheme $k = l = 2$ is A-stable if (Figure 1)

$$B_1 \geq 0 . \tag{13}$$

Eqs. 10 has a singular divergence if

$$\nabla^T f_j(y_{n-1})\, J_f^T(y_{n-1}) f(y_{n-1}) = 0 . \tag{14}$$

In fact, whenever the magnitude $\left|\nabla^T f_j\, J_f^T f\right|$ becomes very small, the coefficient c_j becomes very large, and the numerical solution of the implicit algebraic Eq. 9 fails. A good practical alternative is to switch to the BDF method which is A-stable and $O(h^2)$ (Ascher and Petzold 1998) whenever any of the absolute values of the non-linear terms, $|c_j|$, exceeds a critical threshold. For $k=2$, $B_{i,j}=B_i$ and $A_{i,j}=A_i$, the BDF coefficients are

$$A_0=\frac{3}{2},\ A_1=-2,\ A_2=\frac{1}{2},\ B_0=1,\ B_1=0,\ B_2=0. \tag{15}$$

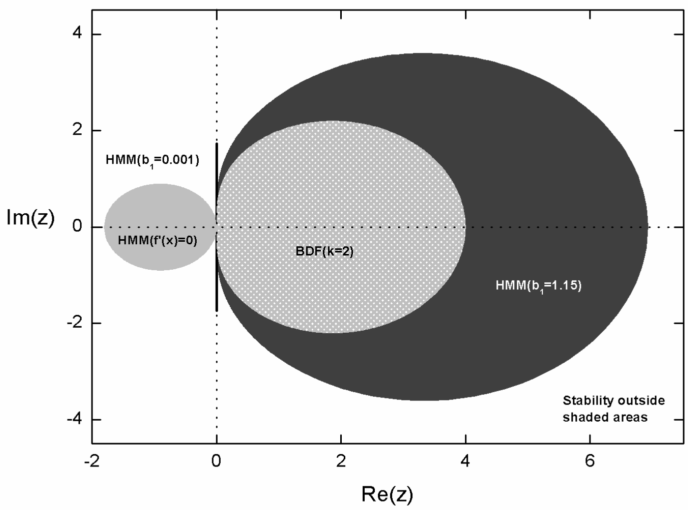

Figure 1. HMM and BDF absolute stability regions.

3 HMM APPLIED TO INDEX-1 DAE

Applying the set of transformations given by Eqs. 7 to Eq. 2, leads to

$$F\left(t,\begin{pmatrix}\sum_{i=0}^{l}A_{i,0}y_{n-i,1}\\ \ldots\\ \sum_{i=0}^{l}A_{i,m}y_{n-i,m}\end{pmatrix},\begin{pmatrix}\frac{1}{h}\sum_{i=0}^{l}B_{i,0}y_{n-i,1}\\ \ldots\\ \frac{1}{h}\sum_{i=0}^{l}B_{i,m}y_{n-i,m}\end{pmatrix}\right)=0\,. \tag{16}$$

The Eq. 16 is similar to Eq. 8, and we can apply the same method to obtain the values of the coefficients. For the values of coefficients according to Eq. 10, the main difference is the non-linear correction term

$$c_j=\frac{\left(f^T H_{f_j}\ f\right)\left(4-3B_{1,j}\right)}{24\left(\nabla^T f_j\ J_f^T f\right)}, \tag{17}$$

since the calculation requires the corresponding Jacobian ∇f and Hessians H_j of f (*i.e.* in Eq. 8 H_j and ∇f are evaluated at $y_{n\text{-}1}$, and $y_{n-1}^{(1)} = f(y_{n-1})$).

However, it is possible to find expressions J_f and H_f

$$J_f = R(F, J_F),\ H_f = S(F, J_F, H_F). \tag{18}$$

Regarding that

$$F_j(y, f(y)) = 0,\ j = 1,\ldots,m, \tag{19}$$

and differentiating Eq. 19 respect to y_k yields

$$\frac{\partial}{\partial y_k} F_j(y, f(y)) + \sum_h \frac{\partial}{\partial y_h^{(1)}} F_j(y, f(y)) \frac{\partial y_h^{(1)}}{\partial y_k} = 0,\ j = 1,\ldots,m. \tag{20}$$

This can be simplified using vectorial notation obtaining

$$\nabla_{F,y} F_j + \nabla_{F,y^{(1)}} F_j J_f = 0, \tag{21}$$

therefore

$$J_f = -\left(J_{F,y^{(1)}} F\right)\left(J_{F,y} F\right). \tag{22}$$

To obtain H_f we should to apply the same kind of formulae considering that $H_{f_j} = J\left(\nabla_{f_j}\right)$. Differentiating Eq. 20 w.r.t. y_r we obtain

$$\begin{aligned} &\frac{\partial}{\partial y_r}\frac{\partial}{\partial y_k} F_j(y, f(y)) + \sum_h \frac{\partial}{\partial y_h^{(1)}}\frac{\partial}{\partial y_k} F_j(y, f(y)) \frac{\partial y_h^{(1)}}{\partial y_r} + \\ &\sum_h \frac{\partial}{\partial y_r}\frac{\partial}{\partial y_h^{(1)}} F_j(y, f(y)) \frac{\partial y_h^{(1)}}{\partial y_k} + \\ &\sum_{h,l} \frac{\partial}{\partial y_l^{(1)}}\frac{\partial}{\partial y_h^{(1)}} F_j(y, f(y)) \frac{\partial y_h^{(1)}}{\partial y_k}\frac{\partial y_l^{(1)}}{\partial y_h} + \\ &\sum_h \frac{\partial}{\partial y_h^{(1)}} F_j(y, f(y)) \frac{\partial^2 y_h^{(1)}}{\partial y_r \partial y_k} = 0, \end{aligned} \tag{23}$$

where $\frac{\partial^2 y_h^{(1)}}{\partial y_r \partial y_k}$ is the (r,k) component of the H_f.

4 NUMERICAL EXPERIMENTS

Two examples were numerically studied solving particular cases of index-1 DAEs. The second example illustrates some of the differences arising when solving DAEs and ODEs.

4.1 Example 1: Unipolar hydrodynamic model for semiconductors

The hydrodynamic model for semiconductor has attracted a lot of attention in both applied mathematics and semiconductor physics (Li 2005). The simplified hydrodynamic model in the case of one carrier type (*i.e.* electrons), called unipolar case also, it can be written as

$$\begin{aligned} &\phi^{(1)} = \delta E - \alpha J, \\ &E^{(1)} = \delta - 1, \\ &J^2 + \delta^2 - \phi\delta = 0, \end{aligned} \tag{24}$$

with initials values $\phi(0) = 3.08$, $E(0) = -1.14$, and $\delta(0) = 0.5\phi(0) + \sqrt{0.25\phi(0)^2 - J^2}$, where $J = 0.5$ and $\alpha = 0.1$ are the parameters or constants. Figure 2 shows the temporal evolution of the variables ϕ, E, and δ.

The corresponding Jacobian and Hessians of f_1, f_2 and f_3 are:

$$J = \begin{bmatrix} 0 & \delta & E \\ 0 & 0 & 1 \\ \frac{(\delta E - 0.05)\delta}{(\phi-2)^2} & \frac{\delta^2}{(\phi-2)} & -\frac{(\delta E - 0.05)\delta}{(\phi-2)} - \frac{\delta E}{(\phi-2)} \end{bmatrix},$$

$$H_{f_1} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, H_{f_2} = 0,$$

$$H_{f_3} = \begin{bmatrix} \frac{2(\delta E - 0.05)\delta}{(\phi-2)^3} & \frac{\delta^2}{(\phi-2)^2} & \frac{(\delta E - 0.05)\delta}{(\phi-2)^2} + \frac{\delta E}{(\phi-2)^2} \\ \frac{\delta^2}{(\phi-2)^2} & 0 & -\frac{2\delta}{(\phi-2)} \\ \frac{(\delta E - 0.05)\delta}{(\phi-2)^2} + \frac{\delta E}{(\phi-2)^2} & -\frac{2\delta}{(\phi-2)} & -\frac{2E}{(\phi-2)} \end{bmatrix}.$$

Figure 3 shows the temporal evolution of the non-linear correction terms c_i. The largest changes of the coefficients occur in the interval for *t* between 0.9 and 1.3 (when $\phi \approx 2$) producing the indeterminacy in the matrix Jacobian *J*, and in the matrix Hessian H_{f_3}.

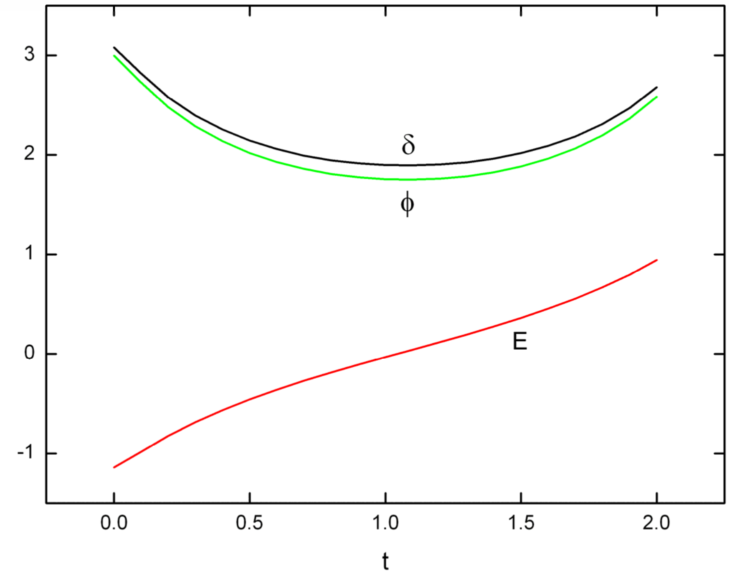

Figure 2. Temporal evolution of the state variables ϕ, E, and δ.

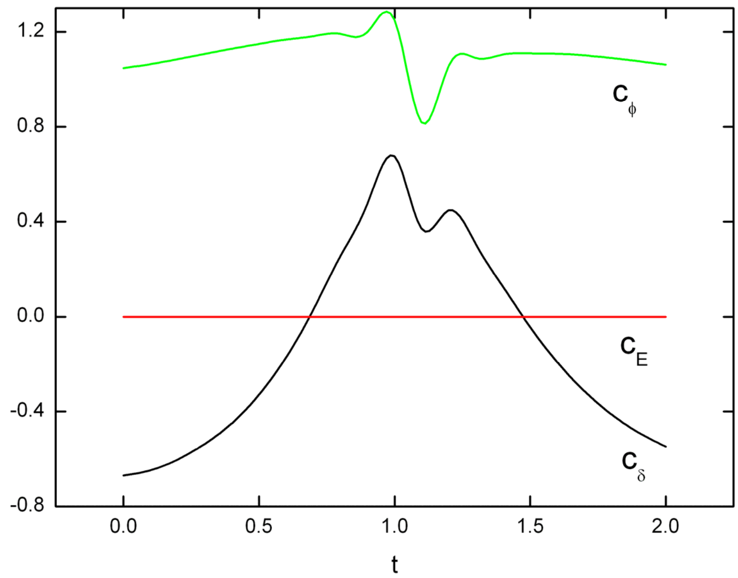

Figure 3. Temporal evolution of the non-linear term c_ϕ, c_E, and c_δ.

4.2 Robertson's problem

The Robertson's problem describes the kinetics of an autocatalytic reaction, and it is commonly used as a test problem in the stiff integrations comparisons (Robertson 1966). The problem consists of a stiff system of 2 nonlinear ODEs and 1 linear algebraic equation:

$$\begin{aligned} y_a^{(1)} &= -k_1 y_a + k_2 y_b y_c , \\ y_b^{(1)} &= k_1 y_a - k_2 y_b y_c - k_3 y_b^2 , \\ 1 &= y_a + y_b + y_c , \end{aligned} \tag{25}$$

with initials values $y_a(0)=1$, $y_b(0)=0$, $y_c(0)=0$, where $k_1 = 0.04$, $k_2 = 10^4$, and $k_3 = 3\cdot 10^7$ are the rate constants. The large difference among the reactions rate constants is the reason for stiffness. Fig. 4 shows the temporal evolution of the variables y_a, y_b, and y_c.

The corresponding Jacobian and Hessians of f_1, f_2 and f_3 are:

$$J = \begin{bmatrix} -0.04 & y_c 10^5 & y_b 10^5 \\ 0.04 & -y_b 6\cdot 10^8 - y_c 10^5 & -y_b 10^5 \\ 0 & y_b 6\cdot 10^8 & 0 \end{bmatrix},$$

$$H_{f_1} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 10^5 \\ 0 & 10^5 & 0 \end{bmatrix}, H_{f_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -6\cdot 10^8 & -10^5 \\ 0 & -10^5 & 0 \end{bmatrix}, H_{f_3} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 6\cdot 10^8 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

The non-linear correction terms are given by:

$$\begin{aligned} c_{y_a} = {} & 6\cdot 10^{11} y_b^2 \left[-0.04 y_a + 10^5 y_b y_c + 3\cdot 10^7 y_b^2\right] / \\ & [\ \left(-0.04 y_a + 10^5 y_b y_c\right)\left(-2.4\cdot 10^6 y_b - 4\cdot 10^2 - 1.6\cdot 10^{-3}\right) \\ & -\left[-0.04 y_a + 10^5 y_b y_c + 3\cdot 10^7 y_b^2\right]\left[\left(6\cdot 10^7 y_b + 10^5 y_c\right) + 4\cdot 10^2 - 6\cdot 10^{11} y_b^2\right] \\ & +3\cdot 10^7 \left[10^5 y_b \left(6\cdot 10^7 y_b + 10^5 y_c\right) + 4\cdot 10^2 y_b\right] y_b^2 \ \ ], \end{aligned}$$

$$c_{y_b} = \Big[\left[-0.04 y_a + 10^5 y_b y_c + 3\cdot 10^7 y_b^2\right]\left[-2.4\cdot 10^6 y_a + 6\cdot 10^{11} y_b y_c + 1.8\cdot 10^{15} y_b^2\right]$$
$$-3\cdot 10^7\left[-4\cdot 10^2 + 10^8 y_b y_c + 3\cdot 10^{12} y_b^2\right] y_b^2 \Big] /$$
$$\Big[\left(-0.04 y_a + 10^5 y_b y_c\right)\left(-2.4\cdot 10^6 y_a - 4\cdot 10^2 - 1.6\cdot 10^{-3}\right)$$
$$-\left[-0.04 y_a + 10^5 y_b y_c + 3\cdot 10^7 y_b^2\right]\left[\left(6\cdot 10^8 y_b + 10^5 y_c\right)^2 + 4\cdot 10^2 - 6\cdot 10^{11} y_b^2\right]$$
$$+3\cdot 10^7\left[10^5\left(6\cdot 10^7 y_b + 10^5 y_c\right) y_b + 4\cdot 10^2 y_b\right] y_b^2 \Big],$$

$$c_{y_c} = \left[-0.04 y_a + 10^5 y_b y_c + 3\cdot 10^7 y_b^2\right]\left[-2.4\cdot 10^6 y_a + 6\cdot 10^{11} y_b y_c + 1.8\cdot 10^{15} y_b^2\right] /$$
$$\Big[-2.4\cdot 10^6 y_b\left(0.04 y_a - 10^5 y_b y_c\right) - 1.8\cdot 10^{15} y_b^4$$
$$+6\cdot 10^7\left(6\cdot 10^7 y_b + 10^5 y_c\right)\left(-0.04 y_a + 10^5 y_b y_c + 3\cdot 10^7 y_b^2\right) y_b \Big].$$

Figure 5a shows the temporal evolution of the non-linear correction terms c_y. Fig. 5b indicates the switching periods when the BDF scheme is applied instead of HMM in order to avoid singularities on c_y. It can be seen that the coefficients vary significantly. Figure 6 shows the absolute difference $\left| y_{\mathrm{ODE}} - y_{\mathrm{DAE}} \right|$ between the numerical solutions obtained solving the case as ODE or DAE (using the same time step $h = 10^{-1}$). In this figure it can be seen that the numerical solution obtained with implicit form ODE is always better than the implicit form DAE.

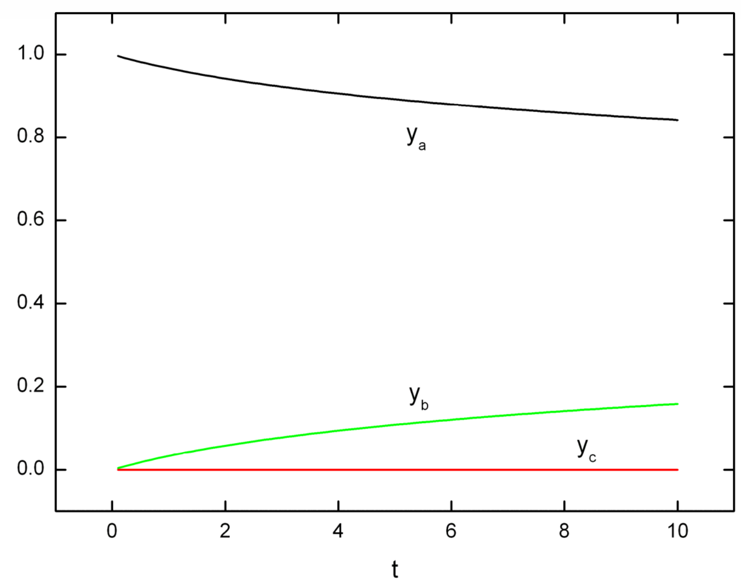

Figure 4. Temporal evolution of the state variables y_a, y_b and y_c.

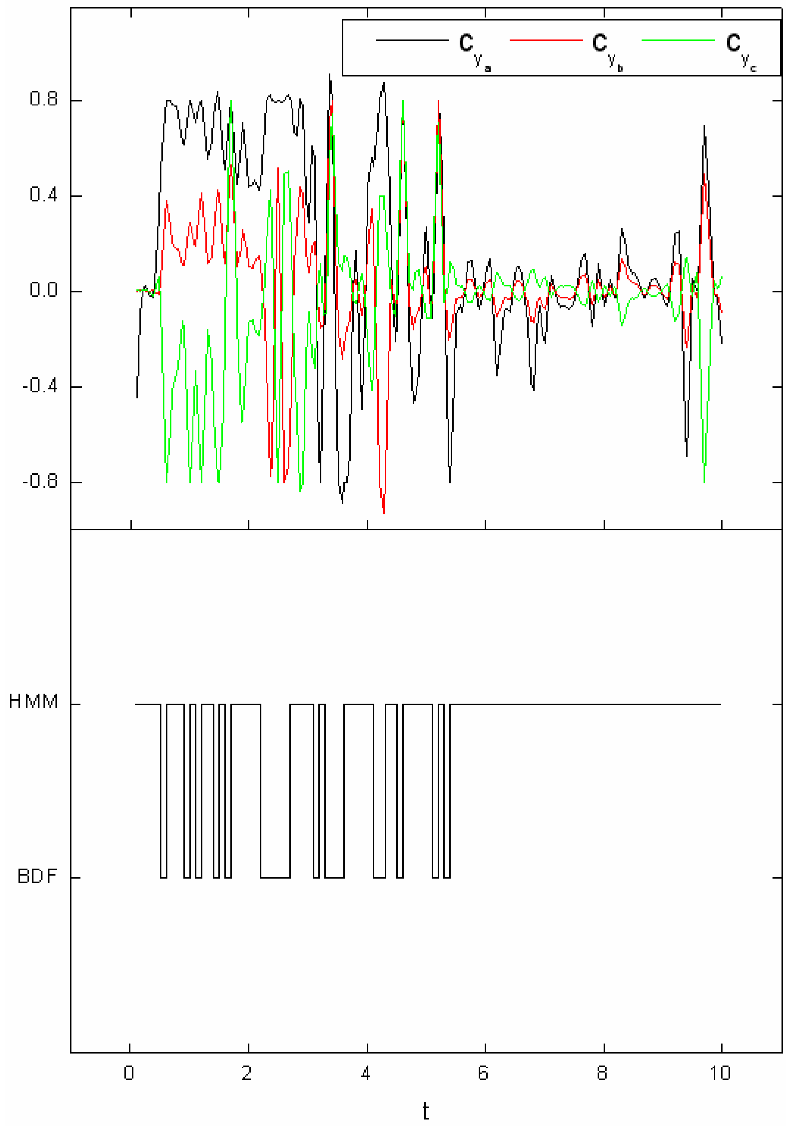

Figure 5. Temporal evolution of the non-linear term c_{y_a} , c_{y_b} and c_{y_c} .

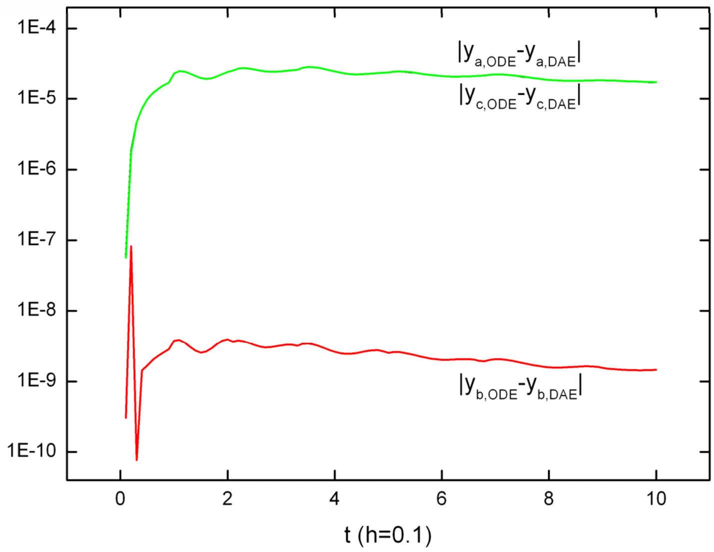

Figure 6. Calculation of the absolute difference $|y_{\mathrm{ODE}} - y_{\mathrm{DAE}}|$ between the numerical solutions obtained for the implicit form ODE and DAE with $h = 10^{-1}$.

5 CONCLUSIONS

A new multistep method to solve index-1 differential-algebraic equations was deduced from an extension of a hybrid linear-nonlinear ODE solver scheme. From the numerical tests we observe as this method may be quite useful for low dimensional problems, like many interesting dynamical systems, where high precision is relevant. For this kind of problems the use of the HMM method gives an interesting alternative to other schemes, namely flexibility on the model implementation in the form of DAE.

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