ONE-LEG INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS WITH GLOBAL ERROR CONTROL\textsuperscript{1}

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Abstract — In this paper we study the family of one-leg two-step second-order methods developed by Dahlquist et al., which possess the $A$-stability and $G$-stability properties on any grid. These methods are implemented with the local-global step size control derived by Kulikov and Shindin with the aim to obtain automatically the numerical solution with any reasonable accuracy set by the user. We show that the error control is more complicated in one-leg methods, especially when applied to stiff problems. Thus, we adapt our local-global step size control for the methods indicated above and test these adaptive algorithms in practice.

2000 Mathematics Subject Classification: 65L05; 65L06; 65L70.

Keywords: one-leg multistep methods, local error evaluation, global error evaluation, stiff problems.

1. Introduction

When applied to ordinary differential equations (ODE’s) of the form

$$x'(t) = g(t, x(t)), \quad t \in [t_0, t_0 + T], \quad x(t_0) = x^0,$$

where $x(t) \in \mathbb{R}^n$ and $g : D \subset \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ is a sufficiently smooth function, the one-leg $l$-step fixed step size method reads

$$\sum_{i=0}^{l} a_i x_{k+1-i} = \tau g \left( \sum_{i=0}^{l} b_i t_{k+1-i}, \sum_{i=0}^{l} b_i x_{k+1-i} \right), \quad k = l - 1, l, \ldots, K - 1. \quad (2)$$

This is a one-leg ”twin” for the conventional $l$-step method

$$\sum_{i=0}^{l} a_i x_{k+1-i} = \tau \sum_{i=0}^{l} b_i g(t_{k+1-i}, x_{k+1-i}), \quad k = l - 1, l, \ldots, K - 1, \quad (3)$$

where $\sum_{i=0}^{l} b_i = 1$. The starting values of $x_k, k = 0, 1, \ldots, l - 1$, of methods (2) and (3) are assumed to be known.

\textsuperscript{1}Part of this work was supported by the National Research Foundation of South Africa
When the step size $\tau$ is fixed both methods will possess the same stability because of the equivalence property [1]. It was the main excuse for introducing one-leg methods since they lead to nonlinear stability ($G$-stability), which is equivalent to $A$-stability [2].

Variable step size versions of methods (2) and (3) have the following form:

$$\sum_{i=0}^{l} a_i(k) x_{k+1-i} = \tau_k g \left( \sum_{i=0}^{l} b_i(k) y_{k+1-i} \right), \quad (4)$$

$$\sum_{i=0}^{l} a_i(k) x_{k+1-i} = \tau_k \sum_{i=0}^{l} b_i(k) g(y_{k+1-i}, x_{k+1-i}), \quad k = l - 1, l, \ldots, K - 1, \quad (5)$$

where $\sum_{i=0}^{l} b_i(k) = 1$. Methods (4) and (5) are no longer equivalent on nonuniform grids and exhibit different stability properties. Nevanlinna and Liniger [11] gave a simple example when the Trapezoidal Rule (multistep method) is unstable, but the Mid-Point Rule (its one-leg twin) is stable for all problems of the form

$$x'(t) = \lambda(t) x(t), \quad \text{Re } \lambda(t) \leq 0$$

and any step size sequences.

For this reason, Dahlquist et al. [3] derived a one-parameter family of one-leg methods that are $A$- and $G$-stable. These methods are a good choice for the variable step size implementation. They have no step size restriction from the point of view of stability. Unfortunately, error control in one-leg methods is quite complicated, which restricts their implementation in practice [4].

Now we want to supply the methods in [3] with the local-global step size control [8] aiming to attain any reasonable accuracy for the numerical solution of problem (1) in automatic mode. We also extend the technique for computing of higher derivatives [9] to the variable-coefficient one-leg methods. It imposes a weaker condition on the right-hand side of problem (1) for the step size selection to be correct, than in [8], where we differentiated interpolating polynomials. We accommodate our local-global control developed for multistep methods in such a way that it works nicely in one-leg two-step methods [3], even for stiff ODE’s of the form (1).

2. Stable one-leg two-step methods

Further, we suppose that ODE (1) possesses a unique solution $x(t)$ on the whole interval $[t_0, t_0 + T]$. To solve problem (1) numerically, we introduce a uniform grid $w_\tau$ with a step size $\tau$ on the interval $[t_0, t_0 + T]$ and apply the $A$- and $G$-stable one-leg method of order 2 in the form

$$\sum_{i=0}^{2} a_i x_{k+1-i} = \tau g \left( \sum_{i=0}^{2} b_i t_{k+1-i} \right), \quad k = 1, 2, \ldots, K - 1, \quad (6)$$

where

$$a_0 \overset{\text{def}}{=} \frac{1}{\gamma + 1}, \quad a_1 \overset{\text{def}}{=} \frac{\gamma - 1}{\gamma + 1}, \quad a_2 \overset{\text{def}}{=} -\frac{\gamma}{\gamma + 1},$$

$$b_0 \overset{\text{def}}{=} \frac{3\gamma + 1}{2(\gamma + 1)^2}, \quad b_1 \overset{\text{def}}{=} \frac{(\gamma - 1)^2}{2(\gamma + 1)^2}, \quad b_2 \overset{\text{def}}{=} \frac{\gamma(\gamma + 3)}{2(\gamma + 1)^2}$$
and the free parameter satisfies the condition $0 < \gamma \leq 1$. Note that we have used a slightly different way to present the family of stable one-leg two-step methods in [3]. The starting values of $x_k$, $k = 0, 1$, are considered to be known.

We apply the following idea in order to fix the parameter $\gamma$. Let us consider the linear test equation $x' = \lambda x$, where $\lambda$ is a complex number. We want to provide the best stability at infinity for method (6). This property is close to the $L$-stability of Ehle [5] and useful when integrating very stiff ODE’s. It means for the one-leg methods (or their multistep twins) that we need to minimize the spectral radius of the companion matrix of method (6) (see [7]).

When $\Re \mu \to -\infty$, the companion matrix of method (6) will have the following form:

$$C_{\infty}(\gamma) \equiv \lim_{\Re \mu \to -\infty} \begin{pmatrix} \frac{\mu b_1 - a_1}{a_0 - \mu b_0} & \frac{\mu b_2 - a_2}{a_0 - \mu b_0} \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -\frac{b_1}{b_0} & -\frac{b_2}{b_0} \\ 1 & 0 \end{pmatrix},$$

where $\mu = \tau \lambda$. Unfortunately, $\rho(C_{\infty}(\gamma)) > 0$ (i.e., the spectral radius of the matrix $C_{\infty}(\gamma)$ is greater than zero) for any $0 < \gamma \leq 1$ because the coefficients $b_1$ and $b_2$ cannot vanish simultaneously (see (6)). Nevertheless, a simple computation shows that the eigenvalues of the matrix $C_{\infty}(\gamma)$ are

$$\lambda_{1,2} = \frac{-(\gamma - 1)^2 \pm (\gamma + 1)\sqrt{\gamma^2 - 18\gamma + 1}}{6\gamma + 2}.$$

Then, we easily calculate that the minimum of the expression $\max\{|\lambda_1|, |\lambda_2|\}$ will be achieved when $\gamma = \gamma_1 \equiv 9 - 4\sqrt{5} \approx 0.055$. Thus, we conclude that $\rho(C_{\infty}(\gamma_1)) = |\lambda_1| = |\lambda_2| = |18 - 8\sqrt{5}|/|3\sqrt{5} - 7| \approx 0.381$.

We note that Dahlquist et al. [3] suggested a different value for $\gamma$. They tried to minimize the error constant of method (6) and preserve good stability properties. Their choice was $\gamma_2 \equiv 1/5$.

Formula (6) implies that the step size $\tau$ must be fixed. The latter requirement is too restrictive for many practical problems. Therefore, we determine continuous extensions to nonuniform grids for both methods of the form of (6) (with the different $\gamma$’s) and come to the following formulas:

$$\frac{\theta_k}{9 - 4\sqrt{5} + \theta_k} x_{k+1} + \frac{\theta_k(8 - 4\sqrt{5})}{9 - 4\sqrt{5} + \theta_k} x_k + \frac{\theta_k(4\sqrt{5} - 9)}{9 - 4\sqrt{5} + \theta_k} x_{k-1}$$

$$= \tau_k g \left( t_{k+1} - \tau_k \theta_k^2 + (2\theta_k + 1)(9 - 4\sqrt{5}) \theta_k^2 + (2\theta_k + 1)(9 - 4\sqrt{5}) \theta_k^2 + (2\theta_k + 1)(9 - 4\sqrt{5}) \theta_k^2 \right) x_{k+1} + (2\sqrt{5} - 4)(\theta_k^2 + 9 + 4\sqrt{5}) (9 - 4\sqrt{5}) (\theta_k^2 + 2\theta_k + 9 + 4\sqrt{5}) (9 - 4\sqrt{5}) x_{k-1} \right) \right),$$

$$\frac{5\theta_k}{1 + 5\theta_k} x_{k+1} - \frac{4\theta_k}{1 + 5\theta_k} x_k - \frac{\theta_k}{1 + 5\theta_k} x_{k-1}$$

$$= \tau_k g \left( t_{k+1} - \tau_k \frac{5\theta_k^2 + 2\theta_k + 1}{2\theta_k(1 + 5\theta_k)} \frac{25\theta_k^2 + 10\theta_k + 5}{2(1 + 5\theta_k)^2} \right) x_{k+1} + \frac{10\theta_k^2 - 2}{(1 + 5\theta_k)^2} x_k + \frac{5\theta_k^2 + 10\theta_k + 1}{2(1 + 5\theta_k)^2} x_{k-1} \right).$$
where \( \tau_k \) is the current step size of the nonuniform grid \( w_x \) with a diameter \( \tau \) (i.e., \( \tau = \max_k \{ \tau_k \} \)) and \( \theta_k = \tau_k / \tau_{k-1} \) is the ratio of adjacent step sizes. We have used our choice for \( \gamma \), i.e. \( \gamma_1 \), in formula (7) and \( \gamma_2 \) to obtain method (8).

3. Errors Estimation for Nonstiff Problems

We recall that both methods (7) and (8) are A- and G-stable on any nonuniform grid. Thus, we control the step sizes by the accuracy requirement alone. With this idea in mind, we impose the following restriction on the step size change:

\[
\frac{\tau}{\tau_{\text{min}}} \leq \Omega < \infty. \tag{9}
\]

We need formula (9) for the local-global step size control to be correct. On the other hand, it does not influence the practical implementation of the error control strategy (see [10] for details).

We further present the theory of local and global errors computation for the one-leg methods (7) and (8) together. So, it is convenient to consider the family of numerical methods [3] in the following general form:

\[
\frac{\theta_k}{\theta_k + \gamma} x_{k+1} + \frac{\theta_k(\gamma - 1)}{\theta_k + \gamma} x_k - \frac{\theta_k \gamma}{\theta_k + \gamma} x_{k-1} = \tau_k g \left( t_{k+1} - \tau_k \frac{2 \theta_k^2 + 2 \theta_k \gamma + \gamma}{2 \theta_k (\theta_k + \gamma)} x_{k+1} + \frac{(1 - \gamma)(\theta_k^2 \gamma - \gamma)}{2(\theta_k + \gamma)^2} x_k \right. \\
+ \left. \frac{\gamma(\theta_k^2 + 2 \theta_k + \gamma)}{2(\theta_k + \gamma)^2} x_{k-1} \right), \tag{10}
\]

where \( \gamma \) is the free parameter, \( \tau_k \) is the most recent step size, and \( \theta_k \) is the current step size ratio.

Following Dahlquist [4], we introduce the defects

\[
L_D(x(t), t_{k+1}, \tau_k) \overset{\text{def}}{=} \sum_{i=0}^{2} a_i(k)x(t_{k+1-i}) - \tau_k g \left( t_{k+1} - \beta(k)\tau_k, x(t_{k+1} - \beta(k)\tau_k) \right), \tag{11}
\]

\[
L_I(x(t), t_{k+1}, \tau_k) \overset{\text{def}}{=} \sum_{i=0}^{2} b_i(k)x(t_{k+1-i}) - x(t_{k+1} - \beta(k)\tau_k), \tag{12}
\]

where \( \beta(k) \overset{\text{def}}{=} \frac{\theta_k^2 + 2 \theta_k \gamma + \gamma}{2 \theta_k (\theta_k + \gamma)} \), and \( a_i(k), b_i(k) \) mean the corresponding coefficients in method (10). Here, (11) is the differentiation defect and (12) is the interpolation one.

By definition of the defects, we have

\[
\sum_{i=0}^{2} a_i(k)x(t_{k+1-i}) = \tau_k g \left( t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)x(t_{k+1-i}) - L_I(x(t), t_{k+1}, \tau_k) \right) + L_D(x(t), t_{k+1}, \tau_k). \tag{13}
\]

Now we subtract (10) from (13) to obtain the following formula for the error \( \Delta x_{k+1} = \)
$x(t_{k+1}) - x_{k+1}, \ i = 0, 1, \ldots, K - 1,$ of method (10):

$$\Delta x_{k+1} \approx \left(a_0(k)I_n - \tau_k b_0(k)\partial_x g\left(t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)x_{k+1-i}\right)\right)^{-1} \times \left(-\sum_{i=1}^{2} a_i(k)\Delta x_{k+1-i} + \tau_k \partial_x g\left(t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)x_{k+1-i}\right)\right) \times \sum_{i=1}^{2} b_i(k)\Delta x_{k+1-i} + L_D(x(t), t_{k+1}, \tau_k)$$

$$- \tau_k \partial_x g\left(t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)x_{k+1-i}\right) L_I(x(t), t_{k+1}, \tau_k).$$

(14)

Here, we have expanded the right-hand side $g\left(t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)(x_{k+1-i} + \Delta x_{k+1-i}) - L_I(x(t), t_{k+1}, \tau_k)\right)$ in the Taylor series at the point $\sum_{i=0}^{2} b_i(k)x_{k+1-i}$ with an accuracy up to the second order terms. We have also neglected any terms of order $O\left(\tau_k \sum_{i=0}^{2} |b_i(k)||\Delta x_{k+1-i}|^2 + ||L_I(x(t), t_{k+1}, \tau_k)||^2\right)$.

For the local error of method (10), we just replace the errors at previous grid points in formula (14) with zeros and come to

$$\Delta \tilde{x}_{k+1} \approx \left(a_0(k)I_n - \tau_k b_0(k)\partial_x g\left(t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)\tilde{x}_{k+1-i}\right)\right)^{-1} \times \left(L_D(x(t), t_{k+1}, \tau_k) - \tau_k \partial_x g\left(t_{k+1} - \beta(k)\tau_k, \sum_{i=0}^{2} b_i(k)\tilde{x}_{k+1-i}\right) L_I(x(t), t_{k+1}, \tau_k)\right),$$

(15)

where the tilde implies that we use the improved numerical solution $\tilde{x}_{k+1} \overset{\text{def}}{=} x_{k+1} + \Delta x_{k+1}$ in formula (15).

We recall that the order of any one-leg method is $s = \min\{s_D, s_I+1\}$ if $L_D(x(t), t_{k+1}, \tau_k) = O(\tau_k^{s_D+1})$ and $L_I(x(t), t_{k+1}, \tau_k) = O(\tau_k^{s_I+1})$ [4]. Therefore we see that the local defects of formulas (14) and (15) is $O(\tau^5)$. Of course, when integrating numerically, we have to take into account the accumulation of the defect of (14) and conclude that the accuracy of the error estimation (14) is $O(\tau^4)$. This result will be correct only if we calculate both defects (11) and (12) with an error of $O(\tau^5)$ at most. Unfortunately, it is quite difficult to achieve this in practice. Thus, we just replace the exact defects $L_D(x(t), t_{k+1}, \tau_k)$ and $L_I(x(t), t_{k+1}, \tau_k)$ with their estimates obtained as follows:

$$L_D(x(t), t_{k+1}, \tau_k) \approx -\frac{3}{6} \left(\sum_{i=0}^{2} a_i(k)\psi_1^3(\theta_k) + 3\beta^2(k)\right) \tilde{x}^{(3)}(t_{k+1}),$$

(16)

$$L_I(x(t), t_{k+1}, \tau_k) \approx \frac{\tau_k^2}{2} \left(\sum_{i=0}^{2} b_i(k)\psi_1^2(\theta_k) - \beta^2(k)\right) \tilde{x}^{(2)}(t_{k+1}),$$

(17)
where \( \psi_0(\theta_k) \equiv 0 \), \( \psi_1(\theta_k) \equiv 1 \), \( \psi_2(\theta_k) = 1 + \theta_k^{-1} \), and \( \ddot{x}^{(j)}(t_{k+1}), j = 2, 3 \), are the numerical derivatives calculated by the improved numerical solution. Note that formulas (16) and (17) are accurate to \( O(\tau^4) \) and \( O(\tau^3) \), respectively.

Thus, formulas (14)–(17) say that we will be in position to calculate the principal terms of the local and global errors of method (10) if we know the derivatives \( x^{(2)}(t_{k+1}) \) and \( x^{(3)}(t_{k+1}) \) with an error of \( O(\tau) \) at most. So, we just refer the reader to [9] for the method to obtain the following approximations:

\[
L_D(x(t), t_{k+1}, \tau_k) \approx \tau_k \sum_{i=0}^{2} c_i^D(k)g(t_{k+1-i}, \bar{x}_{k+1-i}),
\]

\[
L_I(x(t), t_{k+1}, \tau_k) \approx \tau_k \sum_{i=0}^{2} c_i^I(k)g(t_{k+1-i}, \bar{x}_{k+1-i}),
\]

where

\[
c_i^D(k) \overset{\text{def}}{=} \frac{-1}{3} \left( \sum_{i=0}^{2} a_i(k)\psi_i^2(\theta_k) + 3\beta^2(k) \right) q_{2,i+1}^{(2,2)} , \quad i = 0, 1, 2,
\]

\[
c_i^I(k) \overset{\text{def}}{=} \frac{1}{2} \left( \sum_{i=0}^{2} b_i(k)\psi_i^2(\theta_k) - \beta^2(k) \right) q_{2,i+1}^{(2,2)} , \quad i = 0, 1, 2.
\]

We only note that the entries \( q_{2,i+1}^{(2,2)} \) and \( q_{3,i+1}^{(2,2)} \), \( i = 0, 1, 2 \), of the transformation matrix \( Q(2, 2) \) depend on the step size ratio \( \theta_k \) in this paper. Then, trivial calculations produce

\[
c_0^D(k) = \frac{P_1(\theta_k)}{12\theta_k(\theta_k + 1)(\theta_k + \gamma)^2}, \quad c_1^D(k) = \frac{-P_1(\theta_k)}{12\theta_k(\theta_k + \gamma)^2}, \quad c_2^D(k) = \frac{P_1(\theta_k)}{12(\theta_k + 1)(\theta_k + \gamma)^2},
\]

\[
c_0^I(k) = \frac{(2\theta_k + 1)P_1(\theta_k)}{8\theta_k(\theta_k + 1)(\theta_k + \gamma)^2}, \quad c_1^I(k) = \frac{-(\theta_k + 1)P_1(\theta_k)}{8\theta_k^2(\theta_k + \gamma)^2}, \quad c_2^I(k) = \frac{P_1(\theta_k)}{8(\theta_k + 1)(\theta_k + \gamma)^2},
\]

where \( P_1(\theta_k) \overset{\text{def}}{=} \theta_k^4 + 4\gamma \theta_k^3 + 6\gamma^2 \theta_k^2 + 4\gamma \theta_k + \gamma^2 \).

4. Errors Estimation for Stiff Problems

Formulas (14)–(21) will compute quite good estimates for the local error and for the global one when problem (1) is nonstiff. Unfortunately, Dahlquist [4] pointed out that the Jacobi matrix \( \partial_x g(t_{k+1} - \beta(\theta_k)\tau_k, \sum_{i=0}^{2} b_i(k)x_{k+1-i}) \) will have large magnitude eigenvalues when the problem is stiff. The latter leads to numerical instability of the error estimation above and unnecessarily small step sizes. Therefore we show further how to improve formulas (14) and (15) for stiff ODE’s.

We first transform (15) to the following form:

\[
\Delta \bar{x}_{k+1} \approx \left( a_0(k)I_n - \tau_k b_0(k)\partial_x g(t_{k+1} - \beta(\theta_k)\tau_k, \sum_{i=0}^{2} b_i(k)\bar{x}_{k+1-i}) \right)^{-1}
\]

\[
\times \left( L_D(x(t), t_{k+1}, \tau_k) - \frac{a_0(k)}{b_0(k)} L_I(x(t), t_{k+1}, \tau_k) \right) + \frac{1}{b_0(k)} L_I(x(t), t_{k+1}, \tau_k).
\]
Then, replacing the defects in formula (22) with approximations (18) and (19) we arrive at

\[
\Delta \tilde{x}_{k+1} \approx \left( a_0(k) I_n - \tau_k b_0(k) \partial_x g \left( t_{k+1} - \beta(k) \tau_k \sum_{i=0}^{2} b_i(k) \tilde{x}_{k+1-i} \right) \right)^{-1} 
\times \tau_k \sum_{i=0}^{2} c_i(k) g(t_{k+1-i}, \tilde{x}_{k+1-i}) + \tau_k \sum_{i=0}^{2} \tilde{c}_i(k) g(t_{k+1-i}, \tilde{x}_{k+1-i}),
\]

(23)

where the modified coefficients \( c_i(k), \tilde{c}_i(k), i = 0, 1, 2, \) are defined by

\[
c_i(k) \overset{\text{def}}{=} c_i^{D}(k) - \frac{a_0(k)}{b_0(k)} c_i^{l}(k), \quad \tilde{c}_i(k) \overset{\text{def}}{=} \frac{c_i^{l}(k)}{b_0(k)}.
\]

(24)

Formula (23) calculates correctly the principal term of the local error of the one-leg method (10).

The absolutely same reasoning shows that the global error of method (10) satisfies

\[
\Delta \tilde{x}_{k+1} \approx \left( a_0(k) I_n - \tau_k b_0(k) \partial_x g \left( t_{k+1} - \beta(k) \tau_k \sum_{i=0}^{2} b_i(k) x_{k+1-i} \right) \right)^{-1} 
\times \left( \sum_{i=1}^{2} \tilde{a}_i(k) \Delta_1 x_{k+1-i} + \tau_k \sum_{i=0}^{2} c_i(k) g(t_{k+1-i}, \tilde{x}_{k+1-i}) \right) 
- \sum_{i=1}^{2} \tilde{b}_i(k) \Delta_1 x_{k+1-i} + \tau_k \sum_{i=0}^{2} \tilde{c}_i(k) g(t_{k+1-i}, \tilde{x}_{k+1-i}),
\]

(25)

where the coefficients \( c_i(k), \tilde{c}_i(k) \) are calculated by (24) and the modified coefficients \( \tilde{a}_i(k), \tilde{b}_i(k), i = 1, 2, \) are the following:

\[
\tilde{a}_i(k) \overset{\text{def}}{=} \frac{a_0(k)}{b_0(k)} b_i(k) - a_i(k), \quad \tilde{b}_i(k) \overset{\text{def}}{=} \frac{b_i(k)}{b_0(k)}.
\]

(26)

Formula (25) has been designed to compute the principal term of the global error of the methods under consideration.

Using (24) and (26) we easily calculate the modified coefficients for the local and global errors evaluation in method (10) explicitly

\[
c_0(k) = -\frac{P_2(\theta_k)(5\theta_k^2 + (4\gamma + 3)\theta_k + 2\gamma)}{12\theta_k(\theta_k + \gamma)^2(\theta_k + 1)}, \quad \tilde{c}_0(k) = \frac{P_2(\theta_k)(2\theta_k + 1)}{4\theta_k^2(\theta_k + 1)},
\]

\[
c_1(k) = \frac{P_2(\theta_k)(2\theta_k^2 + (\gamma + 3)\theta_k + 2\gamma)}{12\theta_k(\theta_k + \gamma)^2}, \quad \tilde{c}_1(k) = -\frac{P_2(\theta_k)(\theta_k + 1)}{4\theta_k^2},
\]

\[
c_2(k) = -\frac{P_2(\theta_k)(2\theta_k^2 + \gamma\theta_k - \gamma)}{12(\theta_k + \gamma)^2(\theta_k + 1)}, \quad \tilde{c}_2(k) = \frac{P_2(\theta_k)}{4(\theta_k + 1)},
\]

\[
\tilde{a}_1(k) = \frac{2\theta_k^2(1 - \gamma)}{\theta_k^2 + 2\gamma\theta_k + \gamma}, \quad \tilde{b}_1(k) = \frac{(\theta_k^2 - \gamma)(1 - \gamma)}{\theta_k^2 + 2\gamma\theta_k + \gamma},
\]

\[
\tilde{a}_2(k) = \frac{2\gamma\theta_k(\theta_k + 1)}{\theta_k^2 + 2\gamma\theta_k + \gamma}, \quad \tilde{b}_2(k) = \frac{(\theta_k^2 + 2\theta_k + \gamma)\gamma}{\theta_k^2 + 2\gamma\theta_k + \gamma}.
\]
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where

\[
P_2(\theta_k) = \frac{\theta_k^4 + 4\gamma \theta_k^3 + 6\gamma^2 \theta_k^2 + 4\gamma \theta_k + \gamma^2}{\theta_k^2 + 2\gamma \theta_k + \gamma}.
\]

We emphasize that the local and global errors evaluation (23), (25) is recommended to be used for both stiff problems and nonstiff ones. Formulas (14), (15) and (23), (25) are mathematically equivalent and calculate the local and global errors of method (10) with the same accuracy. However, formulas (23), (25) are preferable because they avoid the additional multiplication by the Jacobi matrix, especially when large-scale ODE’s are solved.

To the end, we refer to [8, 10] for the local-global step size control algorithm and for the starting procedure.

5. Numerical Experiments

The first test problem is taken from [6] and has the form

\[
\begin{align*}
x'_{1}(t) &= 2tx_{2}(t)^{1/2}x_{4}(t), & x'_{2}(t) &= 10t \exp\left(5(x_{3}(t) - 1)\right)x_{4}(t), \\
x'_{3}(t) &= 2tx_{4}(t), & x'_{4}(t) &= -2t \ln(x_{1}(t)), & t \in [0, 3]
\end{align*}
\]

with \(x(0) = (1, 1, 1, 1)^T\). Problem (27) possesses the exact solution

\[
x_{1}(t) = \exp(\sin t^2), \quad x_{2}(t) = \exp(5 \sin t^2), \quad x_{3}(t) = \sin t^2 + 1, \quad x_{4}(t) = \cos t^2.
\]

Therefore it is convenient to verify how our adaptive methods with the conventional and modified local and global errors evaluations will reach the required accuracy.

Table 1. Global errors of the original numerical solutions by methods (7) and (8) (with the local-global step size control) for problem (27)

<table>
<thead>
<tr>
<th>Method</th>
<th>(\epsilon_g = 10^{-01})</th>
<th>(\epsilon_g = 10^{-02})</th>
<th>(\epsilon_g = 10^{-03})</th>
<th>(\epsilon_g = 10^{-04})</th>
<th>(\epsilon_g = 10^{-05})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7)c</td>
<td>8.687 \times 10^{-02}</td>
<td>8.663 \times 10^{-03}</td>
<td>7.544 \times 10^{-04}</td>
<td>9.584 \times 10^{-05}</td>
<td>9.084 \times 10^{-06}</td>
</tr>
<tr>
<td>(8)c</td>
<td>7.781 \times 10^{-02}</td>
<td>9.759 \times 10^{-03}</td>
<td>8.789 \times 10^{-04}</td>
<td>7.810 \times 10^{-05}</td>
<td>8.470 \times 10^{-06}</td>
</tr>
<tr>
<td>(7)m</td>
<td>8.193 \times 10^{-02}</td>
<td>8.919 \times 10^{-03}</td>
<td>7.516 \times 10^{-04}</td>
<td>9.621 \times 10^{-05}</td>
<td>9.059 \times 10^{-06}</td>
</tr>
<tr>
<td>(8)m</td>
<td>7.378 \times 10^{-02}</td>
<td>9.811 \times 10^{-03}</td>
<td>8.907 \times 10^{-04}</td>
<td>7.826 \times 10^{-05}</td>
<td>8.470 \times 10^{-06}</td>
</tr>
</tbody>
</table>

Table 2. Global errors of the extrapolated numerical solutions by methods (7) and (8) (with the local-global step size control) for problem (27)

<table>
<thead>
<tr>
<th>Method</th>
<th>(\epsilon_g = 10^{-01})</th>
<th>(\epsilon_g = 10^{-02})</th>
<th>(\epsilon_g = 10^{-03})</th>
<th>(\epsilon_g = 10^{-04})</th>
<th>(\epsilon_g = 10^{-05})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7)c</td>
<td>2.031 \times 10^{-04}</td>
<td>4.083 \times 10^{-06}</td>
<td>8.623 \times 10^{-08}</td>
<td>3.447 \times 10^{-09}</td>
<td>1.082 \times 10^{-08}</td>
</tr>
<tr>
<td>(8)c</td>
<td>1.572 \times 10^{-04}</td>
<td>4.404 \times 10^{-06}</td>
<td>9.329 \times 10^{-08}</td>
<td>8.701 \times 10^{-10}</td>
<td>4.891 \times 10^{-09}</td>
</tr>
<tr>
<td>(7)m</td>
<td>1.828 \times 10^{-04}</td>
<td>4.278 \times 10^{-06}</td>
<td>8.415 \times 10^{-08}</td>
<td>6.956 \times 10^{-09}</td>
<td>1.566 \times 10^{-09}</td>
</tr>
<tr>
<td>(8)m</td>
<td>1.427 \times 10^{-04}</td>
<td>4.438 \times 10^{-06}</td>
<td>9.473 \times 10^{-08}</td>
<td>1.091 \times 10^{-09}</td>
<td>4.221 \times 10^{-09}</td>
</tr>
</tbody>
</table>
The second problem is quite practical. This is the restricted three body problem (see, for example, [6])

\[
\begin{align*}
x_1''(t) &= x_1(t) + 2x_2'(t) - \mu_1 x_1(t) + \mu_2 y_1(t) - \mu_2 y_1(t), \\
x_2''(t) &= x_2(t) - 2x_1'(t) - \mu_1 x_2(t) - \mu_2 y_2(t), \\
y_1(t) &= \left( (x_1(t) + \mu_2)^2 + x_2(t)^2 \right)^{3/2}, \\
y_2(t) &= \left( (x_1(t) - \mu_1)^2 + x_2(t)^2 \right)^{3/2},
\end{align*}
\]

where \( t \in [0, T], \ T = 17.06521656015796255891, \ \mu_1 = 1 - \mu_2 \) and \( \mu_2 = 0.012277471 \). The initial values for problem (28) are: \( x_1(0) = 0.994, \ x_2(0) = 0, \ x_3(0) = 0, \ x_4(0) = -2.00158510637908252240 \). It has no analytic solution, but its solution-path is periodic. Thus, we are also capable to observe the work of both adaptive methods (with different errors estimators) in practice.

Having fixed the global error bounds and computed the local tolerances by the formula \( \epsilon_l = \epsilon_g^{3/2} \), we apply methods (7) and (8) with the local-global step size control based on the local and global errors evaluations from Section 3 and 4 to problems (27) and (28) and come to the data collected in Tables 1–6. Symbol “c” in these tables means that the conventional errors estimation from Section 3 has been used in the step size selection mechanism. Symbol “m” implies that the modified estimator from Section 4 has been implemented.

We see that both choices of the parameter \( \gamma \) in the family of the numerical methods (10) and the errors estimators developed in this paper lead to good results. All adaptive methods compute numerical solutions with the given accuracy. This conclusion is true for the original numerical solutions (see Tables 1, 3) and the extrapolated solutions as well (see Tables 2, 4). We recommend to use the extrapolated solution as a result of numerical integration because of the better accuracy.

We now want to point out that our choice (method (7)), when \( \gamma = 9 - 4\sqrt{5} \), produces the

<table>
<thead>
<tr>
<th>Method</th>
<th>( \epsilon_g = 10^{-01} )</th>
<th>( \epsilon_g = 10^{-02} )</th>
<th>( \epsilon_g = 10^{-03} )</th>
<th>( \epsilon_g = 10^{-04} )</th>
<th>( \epsilon_g = 10^{-05} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7)c</td>
<td>7.388 \times 10^{-02}</td>
<td>7.005 \times 10^{-03}</td>
<td>9.297 \times 10^{-04}</td>
<td>7.547 \times 10^{-05}</td>
<td>9.907 \times 10^{-06}</td>
</tr>
<tr>
<td>(8)c</td>
<td>8.022 \times 10^{-02}</td>
<td>7.349 \times 10^{-03}</td>
<td>7.072 \times 10^{-04}</td>
<td>8.070 \times 10^{-05}</td>
<td>7.470 \times 10^{-06}</td>
</tr>
<tr>
<td>(7)m</td>
<td>8.253 \times 10^{-02}</td>
<td>9.642 \times 10^{-03}</td>
<td>9.726 \times 10^{-04}</td>
<td>9.751 \times 10^{-05}</td>
<td>9.758 \times 10^{-06}</td>
</tr>
<tr>
<td>(8)m</td>
<td>6.761 \times 10^{-02}</td>
<td>7.325 \times 10^{-03}</td>
<td>7.368 \times 10^{-04}</td>
<td>7.389 \times 10^{-05}</td>
<td>7.382 \times 10^{-06}</td>
</tr>
</tbody>
</table>

Table 3. Global errors of the original numerical solutions by methods (7) and (8) (with the local-global step size control) for problem (28)

<table>
<thead>
<tr>
<th>Method</th>
<th>( \epsilon_g = 10^{-01} )</th>
<th>( \epsilon_g = 10^{-02} )</th>
<th>( \epsilon_g = 10^{-03} )</th>
<th>( \epsilon_g = 10^{-04} )</th>
<th>( \epsilon_g = 10^{-05} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7)c</td>
<td>2.375 \times 10^{-03}</td>
<td>2.216 \times 10^{-05}</td>
<td>2.881 \times 10^{-07}</td>
<td>9.139 \times 10^{-09}</td>
<td>1.765 \times 10^{-08}</td>
</tr>
<tr>
<td>(8)c</td>
<td>1.954 \times 10^{-03}</td>
<td>1.997 \times 10^{-05}</td>
<td>4.780 \times 10^{-07}</td>
<td>1.173 \times 10^{-08}</td>
<td>7.730 \times 10^{-09}</td>
</tr>
<tr>
<td>(7)m</td>
<td>2.438 \times 10^{-03}</td>
<td>3.672 \times 10^{-05}</td>
<td>5.192 \times 10^{-07}</td>
<td>1.708 \times 10^{-08}</td>
<td>4.653 \times 10^{-09}</td>
</tr>
<tr>
<td>(8)m</td>
<td>1.689 \times 10^{-03}</td>
<td>2.202 \times 10^{-05}</td>
<td>3.100 \times 10^{-07}</td>
<td>6.122 \times 10^{-09}</td>
<td>1.646 \times 10^{-08}</td>
</tr>
</tbody>
</table>

Table 4. Global errors of the extrapolated numerical solutions by methods (7) and (8) (with the local-global step size control) for problem (28)
Table 5. Average step sizes of methods (7) and (8) (with the local-global step size control) in integrating problem (28)

<table>
<thead>
<tr>
<th>Method</th>
<th>$\epsilon_g = 10^{-01}$</th>
<th>$\epsilon_g = 10^{-02}$</th>
<th>$\epsilon_g = 10^{-03}$</th>
<th>$\epsilon_g = 10^{-04}$</th>
<th>$\epsilon_g = 10^{-05}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7)c</td>
<td>$1.833 \times 10^{-05}$</td>
<td>$5.720 \times 10^{-06}$</td>
<td>$2.086 \times 10^{-06}$</td>
<td>$5.944 \times 10^{-07}$</td>
<td>$2.152 \times 10^{-07}$</td>
</tr>
<tr>
<td>(8)c</td>
<td>$1.477 \times 10^{-05}$</td>
<td>$4.536 \times 10^{-06}$</td>
<td>$1.409 \times 10^{-06}$</td>
<td>$4.761 \times 10^{-07}$</td>
<td>$1.450 \times 10^{-07}$</td>
</tr>
<tr>
<td>(7)m</td>
<td>$1.934 \times 10^{-05}$</td>
<td>$6.707 \times 10^{-06}$</td>
<td>$2.133 \times 10^{-06}$</td>
<td>$6.756 \times 10^{-07}$</td>
<td>$2.137 \times 10^{-07}$</td>
</tr>
<tr>
<td>(8)m</td>
<td>$1.359 \times 10^{-05}$</td>
<td>$4.529 \times 10^{-06}$</td>
<td>$1.438 \times 10^{-06}$</td>
<td>$4.555 \times 10^{-07}$</td>
<td>$1.441 \times 10^{-07}$</td>
</tr>
</tbody>
</table>

Table 6. Execution time (days:hours:min:sec) of methods (7) and (8) (with the local-global step size control) when integrating problem (28)

<table>
<thead>
<tr>
<th>Method</th>
<th>$\epsilon_g = 10^{-01}$</th>
<th>$\epsilon_g = 10^{-02}$</th>
<th>$\epsilon_g = 10^{-03}$</th>
<th>$\epsilon_g = 10^{-04}$</th>
<th>$\epsilon_g = 10^{-05}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7)c</td>
<td>00:32:55</td>
<td>00:41:36</td>
<td>00:35:31</td>
<td>01:54:49</td>
<td></td>
</tr>
<tr>
<td>(8)c</td>
<td>00:38:58</td>
<td>00:46:59</td>
<td>00:00:01</td>
<td>02:11:27</td>
<td></td>
</tr>
<tr>
<td>(7)m</td>
<td>00:22:57</td>
<td>00:25:12</td>
<td>00:50:01</td>
<td>1:10:48:03</td>
<td></td>
</tr>
<tr>
<td>(8)m</td>
<td>00:32:23</td>
<td>00:08:15</td>
<td>00:12:51</td>
<td>02:06:50</td>
<td></td>
</tr>
</tbody>
</table>

required numerical solutions faster, especially when implemented with the step size selection based on the modified estimation of the local and global errors. Notice that the average step sizes are quite similar for both errors evaluation algorithms (compare the data in Table 5). However, the execution time is significantly less when the modified errors estimator has been applied (see Table 6). This confirms the conclusion made at the end of Section 4.

Now we apply methods (7) and (8) to the Van der Pol’s equation

$$x_1'(t) = x_2(t), \quad x_2'(x) = \mu^2 \left( 1 - x_1(t)^2 \right) x_2(t) - x_1(t), \quad t \in [0, 2]$$

(29)

where $x(0) = (2, 0)^T$, and $\mu = 100$. Problem (29) is considered to be very stiff when the parameter $\mu$ is a big number. Despite the small order of the methods under consideration the

Figure 1. The components $x_1$ and $x_2$ of the Van der Pol’s equation calculated by methods (7) and (8) with $\epsilon_g = 10^{-1}$
results obtained are quite promising. The components of the numerical solution of problem (29) are given in Fig. 1. Both methods have produced the same result (up to an error of $10^{-1}$) which completely corresponds to the picture in [7]. Here, we have used the errors evaluation designed for stiff problems.

The final point to mention is that our choice of $\gamma$ (method (7)) has again computed the numerical solution of the Van der Pol’s equation faster. This is a good reason to implement it in practice.

References