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K-Step Block Predictor-Corrector Methods for Solving First Order Ordinary Differential Equations

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Abstract: A k-step block Predictor-Corrector Methods for solving first Order Ordinary Differential Equations (ODEs) are formulated and applied on non-stiff and mildly stiff problems using variable step size technique. In this method, collocation and interpolation of the power series as the approximate solution is carried out with aim of generating the continuous scheme. The investigation of some selected theoretical properties of the method is analyzed as well as determination of the region of absolute stability of the method. In addition, the implementation of the proposed method is done by applying variable step size technique.

Key words: Predictor-Corrector Method, non-stiff and mildly stiff ordinary differential equations, interval of absolute stability, collocation, variable

INTRODUCTION

The numerical result for Ordinary Differential Equations (ODEs) have great grandness in scientific and technological computation as they were broadly used to framework in presenting the real life problems such as motion of the projectiles or orbiting bodies, population growth, chemical kinetics and economic growth as in (Majid *et al*., 2006). According to James and Adesanya (2014), many practical problems are modelled into first order Ordinary Differential Equations (ODEs) while some that are modeled into second and third order ODEs are computed by reducing them to a system of first order ODEs, thereby resolving with one-step method such as Taylor series, Euler's and Runge-Kutta Methods. Therefore, the subject of first order ODEs is vital. This study views a computational k-step block predictor-corrector with variable step size technique of solving first order initial value problems of ODEs of the form (James and Adesanya, 2014):

$$y' = f(x, y),\ y(a) = y_0,\ a \le x \le b \qquad (1)$$

where, $y'=f(x,y)$ is given a real valued function in the interval $[a, b]\subset[-\infty, \infty]$ which is existed and bounded within the region. We assumed that f(x, y) satisfies Lipchitz conditions that assured the existence and uniqueness of the result to Eq. 1.

Majid *et al*. (2006), iterated that differential equations are frequently utilized to framework or model the real life problems and sometimes these equations do not possess analytic solutions. Thus, a suitable computational method is needed to solve Eq. 1. In Ismail *et al*. (2009), it was reported that other methods exist for providing solution to Eq. 1 but such methods will only estimate the numerical solution at one point consecutively. James and Adesanya (2014) stated that the main disadvantage of the Predictor-Corrector Method is the high cost of execution as subprograms are very difficult to code due to the separate methods needed to provide initial values. Hence, we desire to address this shortcoming by suggesting a method that combines the features of the block method and the Predictor-Corrector Method as well as quicker method that can give better solution to the problem numerically.

Researchers expressed that block methods are one of the computational methods which have been proposed such as Fatunla (1991), James and Adesanya (2014), Biasa *et al*. (2011), Majid *et al*. (2006) and Majid and Suleiman (2007). Notable advantage of block methods is that at each step of the implementation one can get approximate solution in more than one point. In addition, the number of points relies on the formulation of the block method as by Mehrkanoon *et al*. (2010). Consequently, employing these methods can yield quicker solution to the problem and likewise can be managed to bring out the desired accuracy. Ismail *et al*. (2009) and Biasa *et al*. (2011) proposed block Predictor-Corrector Methods for solving first order ODEs using variable step size. Basically, the block Predictor-Corrector Method was initiated to handle stiff ODEs and contrary to James and Adesanya (2014) which was formulated to solve non-stiff

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ODEs using fixed step size. This study is motivated by the fact very few work have been done in solving non-stiff and mildly stiff ODEs using k-step block predictor-corrector employing variable step size technique. In reality, the implementation here follows Milne's Method.

METHODOLOGY

We first state the theorem that demonstrates the sufficient conditions for a unique solution to exist and always assume that the hypotheses of this theorem are satisfied.

Theorem 1: Let f (x, y) be continuous for all (x, y) in a region D = $\{0 \le x \le b, |y| < \infty\}$. Moreover, assume Lipschitz continuity in y; there exists a constant L such that for all (x, y) in D:

$$|f(x, y) - f(x, \bar{y})| \le L|y - \bar{y}|$$

Then, for any $c \in R^m$ there exists a unique solution y (x) throughout the interval [0, b] for the IVP (Eq. 1). This solution is differentiable. The solution y depends continuously on the initial data: if $\bar{y}$ also satisfies the ODE (but not the same initial values) then $|y(x) - \bar{y}(x)| \le e^{Lt}|y(0) - \bar{y}(0)|$.

Thus, we have solution existence, uniqueness and continuous dependence on the data. In other words, a well posed problems-provided that the conditions of the theorem holds (David, 1967).

Theorem 2: The Weierstrass approximation theorem states that a continuous function f(x) over a closed interval [a, b] can be approximated by a polynomial $P_n(x)$, [a, b] of degree n such that $|f(x) - P_n(x)| < \varepsilon x \in [a, b]$. Where $\varepsilon > 0$ is a small quantity and n is sufficiently large (Jain *et al*., 2007).

Theoretical procedure: In this study, we seek a solution (Eq. 1) and this solution may written as:

$$\sum_{i=0}^{i} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i} \tag{2}$$

where, $f_{n+i} \equiv f(x_{n+i}, y_{n+i})$, α_i and β_i are constant and assume that $\alpha_i \ne 0$, $|\alpha_0| + |\beta_0| > 0$. Since, Eq. 2 can be multiplied by the same constant without altering the relationship α_i and β_i are arbitrary to the extent of a multiplication constant. The arbitrariness has been removed by assuming that $\alpha_j = 1$. Method (Eq. 2) is explicit if $\beta_j = 0$ and implicit if $\beta_j = 0$. Generally, implicit methods are solved by iteration as by Lambert (1997).

This study is focused on the use of Milne's Method of variable step technique in developing a type of k-step block Predictor-Corrector Methods for solving first order ODEs forthwith. The method will be formulated based on interpolation and collocation approach using power series as the approximate solution of the problem. Thus, power series approximate solution can be written in the form of:

$$y(x) = \sum_{i=0}^{j} \alpha_i \left(\frac{x - x_i}{h}\right)^i \tag{3}$$

Formulation of the method: According to Lee (2000) in a 2-point block method, the interval [a, b] is divided into subintervals of blocks with each interval containing two points, i.e., x_n and x_{n-1} in the first block while x_{n+1} and x_{n+2} in the second block where solutions to Eq. 3 are to be computed. The method will formulate two new evenly spaced solution values concurrently. Similarly, this can be extended to a 3-point one block method where the backward and forward values are the points of interpolation and collocation as well as evaluation.

Representation of r-point block method: From Fatunla (1991) the r-point block method for Eq. 2 is given by the matrix finite difference equation:

$$A^{(0)}Y_m = \sum_{i=0}^{j} A^{(i)}Y_{m-i} + h\sum_{i=0}^{j} B^{(i)}F_{m-i} \tag{4}$$

$$Y_m = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ . \\ . \\ . \\ y_{n+r} \end{bmatrix}, Fm = \begin{bmatrix} f_{n+1} \\ f_{n+2} \\ . \\ . \\ . \\ f_{n+r} \end{bmatrix} \text{(for n = mr, m = 0, 1, ...)}$$

where, $A^{(i)}$ and $B^{(i)}$ r×r matrices. It is assumed that matrix finite difference equation is normalized so that $A^{(0)}$ is an identity matrix. The block scheme is explicit if the coefficient matrix $B^{(0)}$ is a null matrix. This is performed by approximating Eq. 2 using Eq. 3 with the idea of interpolation and collocation method (it can be described by matrix finite difference equation stated above).

Derivation of r-step Explicit Block Multistep (EBM): As by James and Adesanya (2014), interpolating Eq. 3 at $x = x_n$ and collocating Eq. 3 at $x = x_{n-i}$ for i = 0(1)2 gives a system of equations which can be expressed as AX = U.

Solving for a'_is and substituting the values of a'_is into Eq. 3 gives a continuous scheme Linear Multistep Method in the form:

$$y(x) = \sum_{i=0}^{j} \alpha_i y_{n+i} + h\sum_{i=0}^{j} \beta_i f_{n+i} \quad (5)$$

Evaluating Eq. 5 at points $x = x_{n+i}$ at $i = 1(1)3$, we obtain the convergent k-step explicit block multistep method as:

$$\begin{aligned} y_{n+1} &= y_n + h\left[\frac{23}{12}f_n - \frac{4}{3}f_{n-1} + \frac{5}{12}f_{n-2}\right] \\ y_{n+2} &= y_n + h\left[\frac{19}{3}f_n - \frac{20}{3}f_{n-1} + \frac{7}{3}f_{n-2}\right] \\ y_{n+3} &= y_n + h\left[\frac{57}{4}f_n - 18f_{n-1} + \frac{27}{4}f_{n-2}\right] \end{aligned} \quad (6)$$

According to Fatunla (1991), the k-step explicit block multistep method can be written in matrix finite difference equation as:

$$A^{(0)}Y_n = A^{(1)}Y_{n-1} + hB^{(1)}F_{n-1} \quad (7)$$

Derivation of r-implicit block multistep method: Interpolating (Eq. 3) at $x = x_{n-1}$ and collocating (Eq. 3) $x = x_{n+i}$ for $i = 0(1)3$ gives a system of equations which can be expressed as AX = U (James and Adesanya, 2014).

Solving for a'_is and substituting values of a'_is into Eq. 3 yields a continuous scheme Linear Multistep Method in the form:

$$y(x) = \sum_{i=0}^{j} \alpha_i y_{n+i} + h\sum_{i=0}^{j} \beta_i f_{n+i} \quad (8)$$

Evaluating Eq. 8 at points $x = x_{n+i}$ at $i = 1(1)j$, we obtain the convergent k-step implicit block multistep method as:

$$\begin{aligned} y_{n+1} &= y_{n-1} + h\left[\frac{19}{3}f_{n+1} - \frac{20}{3}f_{n+2} + \frac{7}{3}f_{n+3}\right] \\ y_{n+2} &= y_{n-1} + h\left[\frac{27}{4}f_{n+1} - 6f_{n+2} + \frac{9}{4}f_{n+3}\right] \\ y_{n+3} &= y_{n-1} + h\left[\frac{20}{3}f_{n+1} - \frac{16}{3}f_{n+2} + \frac{8}{3}f_{n+3}\right] \end{aligned} \quad (9)$$

Again, the k-step implicit block multistep method can be written in matrix finite difference equation as (Fatunla, 1991):

$$A^{(0)}Y_m = A^{(1)}Y_{m-1} + h[B^{(0)}F_m] \quad (10)$$

Investigation of the basic properties of the methods

Order of the method

Definition 1: From Lambert (1977), the Linear Multistep Method Eq. 6 and 9 and the associated difference operator:

$$L[y(x); h] = \sum_{i=0}^{j} [\alpha_i y(x+ih) - h\beta_i y'(x+ih)]$$

are said to be of order p if in $L[y(x); h] = C_0 y(x) + C_1 hy'(x) + \ldots + h_q C_q(x)\ y'^q(x) + \ldots$, $C_0 = C_1 = \ldots = C_q = 0$, $C_{p+1} \neq 0$. Following, Jain *et al*. (2007) and Mohammed *et al*. (2013), we observed that the block multistep method of Eq. 6 and 9 has order p, if $C_0 = C_1 = \ldots = C_q = 0$, $C_{p+1} \neq 0$.

Therefore, we concluded that the methods Eq. 6 and 9 have order p = 3 and error constants given by the vectors:

$$C_4 = \left[\frac{3}{8}, \frac{8}{3}, \frac{75}{8}\right]^T$$

And:

$$C_4 = \left[-\frac{8}{3}, -\frac{21}{8}, -\frac{8}{3}\right]^T$$

Convergence

Theorem 1: According to Hairer *et al*. (1987), if the multistep method:

$$y(x) = \sum_{i=0}^{j} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i}$$

is convergent, then it is necessarily:

- Stable
- Consistent (i.e. of order 1: $\rho(1) = 0$, $\rho(1) = \sigma(1)$)

Zero stability

Theorem 1 (first root condition): From Bruce (2007), the multistep methods:

$$y(x) = \sum_{i=0}^{j} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i}$$

is stable if all the roots r_i of the characteristic polynomial $\rho(r)$ satisfy $|r_i| \leq 1$ and $|r_i|$ if then r_i must be a simple root.

Definition 2: As in Hairer *et al*. (1987), the multistep method:

$$y(x) = \sum_{i=0}^{j} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i}$$

is called stable, if the generating polynomial $\rho(r) = \det(r A^{(0)} - E)$ satisfies the first root condition, i.e.:

- The roots of $\rho(r)$ lie on or within the unit circle
- The roots on the unit circle are simple

In order to analyze the methods for zero-stability, Eq. 6 and 9 are both normalize and written as a block method given by the matrix finite difference equations as by Mohammed *et al.* (2013):

$$A^{(0)} = A^{(1)}y_{m-i} + hB^{(1)}f_{m-i}$$

$$A^{(0)} = A^{(1)}y_{m-i} + hB^{(0)}f_m$$

In addition, the zero stability is concerned with the stability of the difference system in the limit as h tends to zero. Thus as $h\to 0$, $\rho(r) = r^{z-\sigma}(r-1)^{\sigma}$ where σ is the order of the differential equation, z is the order of the matrix $A^{(0)}$ and E (Mohammed *et al.*, 2013; Awari, 2013). For our method:

$$\rho(r) = \left[r\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix} - \begin{bmatrix}0&0&1\\0&0&1\\0&0&1\end{bmatrix}\right] = 0$$

$\rho(r) = r^2(r-1)^1$; hence our method is zero stable according to Hairer *et al.* (1987).

Consistency

Theorem 2: According to Bruce (2007), a Linear Multistep Method is consistent if it has order greater than or equal to 1. Thus:

$$\sum_{i=0}^{j} a_i = 0$$

And:

$$\sum_{i=0}^{j} ia_i + \sum_{i=0}^{j} b_i = 0$$

In terms of the characteristic polynomial, the method is consistent if and only if $\rho(1) = 0$, $\rho(1) = \sigma(1)$.

Definition 3: The Linear Multistep Method:

$$\sum_{i=0}^{j} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i}$$

is said to be consistent provided its error order p satisfies $p\geq 1$. It can be shown that this implies that the first and second characteristics polynomial are fulfilled.

$$\rho(1) = 0,\ \rho'(1) = \sigma(1)$$

Since, the block multistep methods Eq. 6 and 9 are consistent as it has order $p>1$. Adopting, Hairer *et al.* (1987), we can conclude the convergence of the block multistep methods Eq. 6 and 9.

Region of absolute stability

Theorem 4 (second root condition): From Bruce, the Linear Multistep Method:

$$\sum_{i=0}^{j} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i}$$

is absolutely stable if all the roots r_i of the characteristic polynomial $\phi(r) = \rho(r) - z\sigma(r)$ satisfy $|r_i| \leq 1$.

Definition: Adesanya *et al.* (2013) and Lambert (1991) the Linear Multistep Method:

$$\sum_{i=0}^{j} \alpha_i y_{n+i} = h\sum_{i=0}^{j} \beta_i f_{n+i}$$

for given $\bar{h}$ if for that $\bar{h}$ all the roots of the stability polynomial $\pi(r; h) = \rho(r) - \bar{h}\sigma(r)$ satisfy $|r_i|<1$, i = 1, 2, .., j where $\bar{h} = \lambda h$ and $\lambda = \partial f/\partial y$.

However, we adopted the boundary locus method to determine the interval of absolute stability of the block methods and to obtain the roots of absolute stability, we substitute the test equation $y = -\lambda y$ into the block formula to obtain:

$$\rho(r) = \det\left(A^{(0)}Y_m(r) - A^{(1)}Y_{m-1}(r) - \left(B^{(1)}F_{m-1}(r)h\lambda\right)\right) = 0 \quad (11)$$

Substituting $\bar{h} = 0$ in Eq. 11, we obtain all the roots of the derived equation to be equal to 1; hence, according to Bruce (2007) defined on theorem 4, the block methods is absolutely stable. Therefore, the boundary of the region of absolute stability is given by:

$$\bar{h}(r) = \frac{\rho(r)}{\sigma(r)} = \frac{r^2-1}{\frac{19}{3}r - \frac{20}{3}r^2 + \frac{7}{3}r^3} \quad (12)$$

Let, $r = e^{i\theta} = \cos\theta + i\sin\theta$, therefore Eq. 1 becomes:

$$\bar{h}(\theta) = \frac{\cos 2\theta - 1}{\frac{19}{3}\cos\theta - \frac{20}{3}\cos 2\theta + \frac{7}{3}\cos 3\theta} \quad (13)$$

Evaluating Eq. 13 at 30° within [0°, 180°] which gives the stability interval to be [-1.075747112, 0] after evaluation at interval of $\bar{h}(\theta)$. The stability interval is shown in Fig. 1.

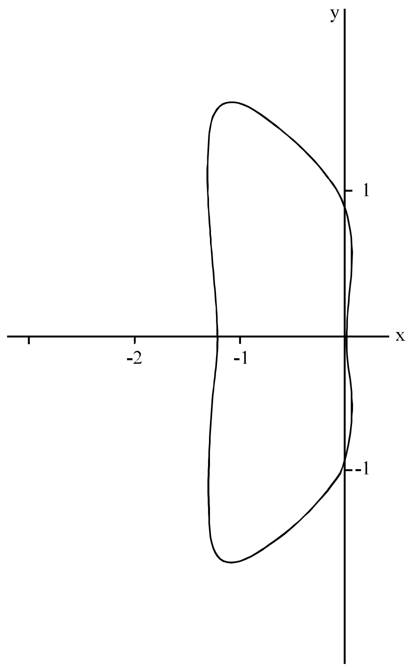

Fig. 1: The region of absolute stability of the block method

Implementation of the variable step-size method: Adopting, Faires and Burden (2012):

- Predictor-corrector techniques always generate two approximations at each step, so they are natural candidates for error-control adaptation
- To demonstrate the error-control procedure, a variable step-size Predictor-Corrector Methods using 3-step Adams-Bashforth Method as predictor and the corrector method using the 2-step Adams-Moulton Method as corrector is constructed

To proceed further, we must make the assumption that for small values of h:

$$y^{(iv)}(\overline{x}) = y^{(iv)}(\tilde{x})$$

If we subtract the (block predictor) local truncation error estimate from the (block corrector) local truncation error estimate and further simplification, we arrive at the approximation to the Adams-Moulton local truncation as:

$$\in^{c}_{n+1} \approx \left|y^{c}_{n+1} - y^{p}_{n+1}\right| = \delta < \varepsilon \qquad (14)$$

Equation 14 is called Milne's estimate. As in Zarina *et al.* (2007), varying the step size is crucial for the effective performance of a discretization method. Step size adjustment for r-point block multistep method using variable step has been stated earlier. On the given step, the user will provide an error tolerance limit. In the block multistep, variable step-size strategy codes, the block solutions are accepted if the local truncation error, LTE is less than the tolerance limit. The LTE is obtained by taking Eq. 14 for n = 1, 2, ..., j where y^{c}_{n+1} and y^{p}_{n+1} represents the predicted and corrected approximation given by the 3-step Adams-Bashforth and 2-step Adams-Moulton Methods while δ is called the convergence test and ε is the tolerance limit. If the error estimate is greater than the accepted tolerance limit, the value of y_{n+1} is rejected, the step is repeated with halving the current step size or otherwise, the step is multiply by 2. The error controls for the code was at the first point in the block because in general it had given us better results according to the new method. The error estimate ($\in^{c}_{n+1}$) is used to decide finally whether to accept the results of the current step or to redo the step with a smaller step size. According to Uri and Linda, the step is accepted based on test displayed previously. Furthermore, Eq. 14 guarantees the convergence of the method during the test evaluation.

NUMERICAL EXPERIMENTS

The performance of the block Predictor-Corrector Method was carried out on non-stiff and mildly stiff problems. For problem 1 and 2 the following tolerances 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, 10^{-10} and 10^{-12} was used to compare the performance of the newly proposed method with other existing methods as by James and Adesanya (2014) (Table 1 and 2).

Table 1: Numerical results by James and Adesanya (2014) and kBPC for solving problem 1

X	Maximum errors	Tolerance levels	Maximum errors
0.1	6.82121 (-13)	10^{-4}	1.42882 (-4)
0.2	2.04636 (-12)	-	-
0.3	2.27373 (-13)	10^{-6}	8.25471 (-7)
0.4	1.13686 (-12)	-	-
0.5	4.54747 (-13)	10^{-8}	8.63637 (-9)
0.6	2.27373 (-13)	-	-
0.7	3.18323 (-12)	10^{-10}	9.44962 (-11)
0.8	4.54747 (-13)	-	-
0.9	9.09494 (-12)	10^{-12}	1.11022 (-16)
1.0	2.04636 (-12)	-	-

Table 2: Numerical results by Mehrkanoon *et al.* (2012) and kBPC for solving problem 2

TOL	MTH	MAXE
10^{-2}	3PG	1.0×10^{-4}
	KBPC	1.32359×10^{-5}
10^{-4}	3PG	9.57×10^{-7}
	KBPC	4.29533×10^{-9}
10^{-6}	3PG	6.64×10^{-9}
	KBPC	6.81677×10^{-14}
10^{-8}	3PG	7.46×10^{-11}
	KBPC	3.33067×10^{-16}
10^{-10}	3PG	5.64×10^{-13}
	KBPC	2.22045×10^{-16}

Tested problems

Problem 1: The first problem to be discussed is extracted from James and Adesanya (2014). Moreover, a note on the construction of constant order predictor corrector algorithm for the solution of first order ODEs was developed and implemented using fixed step size. The newly proposed method is formulated to solve non-stiff and mildly stiff odes using variable step size technique.

The SIR Model is an epidemiological model that computes the theoretical numbers of people infected with a contagious illness in a closed population over time. The name of this class of models derives from the fact they involves coupled equations relation the number of Susceptible people S(t), number of people Infected l(t) and the number of people who have Recovered R(t). Scholars defines this model as good and simple for many infectious diseases including measles, malaria Ebola and so on. The SIR Model is described by the three coupled equations:

$$\frac{ds}{dl} = \mu(I\text{-}S)\text{-}\beta IS$$

$$\frac{dI}{dl} = I(\mu\text{-}\gamma)+\beta IS$$

$$\frac{dR}{dl} = \text{-}\mu R\text{-}\gamma I$$

where, μ, γ and β are positive parameters. Define y to be:

$$y = S+I+R$$

Combining the equations by adding all together, the three coupled equations above becomes:

$$\frac{dy}{dt} = \mu(1\text{-}y)$$

Taking $\mu = 0.5$ and attaching an initial condition $y(0) = 0.5$ (for a closed population), we get:

$$\frac{dy}{dt} = 0.5(1\text{-}y),\ y(0) = 0.5$$

whose exact solution is:

$$y(t) = 1\text{-}0.5e^{-0.5t}$$

Problem 2: Problem 2 was extracted from Ming-Gong. The 3-point implicit block multistep method for the solution of first order odes was designed and implemented using variable step size technique. Moreover, this scheme belong to the Backward Differentiation Formula solely an implicit scheme for solving stiff odes. The newly proposed method belongs to the family of Adams and was created to solve non-stiff and mildly stiff odes. Negative exponential problem (mildly stiff):

$$y' = \text{-}0.5,\ y(0) = 1,\ [a, b] = [0, 20]$$

The exact solution is given by $y(x) = e^{-0.5x}$. The following notational systems are used in the tables:

- TOL: Tolerance
- MTD: Method employed
- MAXE: Magnitude of the Maximum error of the computed solution
- KBPC: K-step Block Predictor-Corrector Method

The following notational systems are used in the tables:

- TOL: Tolerance
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CONCLUSION

From Table 1 (James and Adesanya, 2014) was implemented using fixed step size which does not allow for step size changes, error control and minimization. Hence, the newly proposed method is preferable with the above mentioned. Again from Table 2 (Mehrkanoon *et al*., 2012) was also executed using variable step size which belongs to the family of backward differentiation formula specifically designed to solve stiff ODEs while kBPC is formulated as well to compute non-stiff and mildly stiff ODEs. Moreover, problem solved is based on mildly stiff ODEs. This gives a better result at all tested tolerance levels.

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