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ScienceDirect
Journal of the Nigerian Mathematical Society 34 (2015) 160–168
Journal of the Nigerian Mathematical Society
www.elsevier.com/locate/jnnms

A family of Continuous Third Derivative Block Methods for solving stiff systems of first order ordinary differential equations

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Received 16 August 2014; received in revised form 11 March 2015; accepted 16 June 2015
Available online 27 June 2015

Abstract

This paper presents a family of Continuous Third Derivative Block Methods (CTDBM) of order $k + 3$ for the solution of stiff systems of ordinary differential equations. The approach uses the collocation and interpolation technique to generate the main Continuous Third Derivative method (CTDM) which is then used to obtain the additional methods that are combined as a single block methods. Analysis of the methods show that the method is L-stable up to order eight. Numerical examples are given to illustrate the accuracy and efficiency of the proposed method.

Keywords: Third derivative; Block method; Stability; ODE

1. Introduction

Consider the first order ordinary differential equation

$$y' = f(t, y)\ y(t_0) = y_0. \tag{1}$$

Eq. (1) occurs in several areas of engineering, science and social sciences. It is well known that some of these problems have proved to be either difficult to solve or cannot be solved analytically, hence the necessity of numerical techniques for such problems remains vital. Many physical problems are modeled into first order problem (1), while those modeled in higher order differential equations are either solved directly or solved by first reducing them to system of first-order differential equations. There are various methods available for solving systems of first order IVPs [1,2]. Linear multistep methods for the solution of (1) have been developed varying from discrete linear multistep method to continuous ones. Continuous linear multistep methods have greater advantages over the discrete methods such that they give better error estimation, provide a simplified form of coefficients for further evaluation at different points, and provides solution at all interior points within the interval of integration, (see [3,4]). These methods are first derivative methods that are implemented in predictor corrector mode, and Taylor series expansion are adopted

Peer review under responsibility of Nigerian Mathematical Society.
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http://dx.doi.org/10.1016/j.jnnms.2015.06.002

to supply starting values. The setback of the predictor–corrector methods are that they are very costly to implement, longer computer time and greater human effort and reduced order of accuracy, which affect the accuracy of the method. Second derivative methods have been proposed by Enright [5], Ismail [6], Hojjati [7]. Recently Ezzeddine and Hojjati [8] proposed third derivative method of order $k + 3$. These methods are implemented in a step-by-step fashion in which on the partition Γ, an approximation is obtained at t_{n+1} only after an approximation at t_n has been computed, where $\Gamma : a = t_0 < t_1 < \cdots < t_N = b$, $t_{n+1} = t_n + hn = 0, 1, \ldots, N - 1$ $h = \frac{b-a}{N}$ is the constant step-size of the partition of Γ, N is a positive integer, and n is the grid index. High-order continuous third derivative formulas with block extensions have also been proposed by Jator et al. [9] for the direct solution of the general second order ordinary differential equations. In this paper, a family of Continuous Third Derivative Block Method (CTDBM) that will not only be self starting but are also of good accuracy and have stability properties for effective and efficient solution of stiff system of ordinary differential equations of the form (1) is proposed.

2. Derivation of the method

In this section, a k-step third derivative method of the form

$$y_{n+k} = y_{n+k-1} + h\sum_{j=0}^{k} \alpha_j(t) f_{n+j} + h^2 \beta_k g_{n+k} + h^3 \eta_k \gamma_{n+k} \tag{2}$$

is developed for (1) on the interval from t_n to t_{n+k}.

The initial assumption is that the solution on the interval $[t_n, t_{n+k}]$ is locally approximated by the polynomial

$$Y(t) = \sum_{j=0}^{k+3} \tau_j t^j, \tag{3}$$

where τ_j are unknown coefficients. Since this polynomial must pass through the interpolation points (t_{n+k-1}, y_{n+k-1}) and the collocation points $(t_n, y_n, t_{n+1}, y_{n+1}), \ldots (t_{n+k}, y_{n+k})$, we require that the following $(k + 4)$ equations must be satisfied.

$$\sum_{j=0}^{k+3} \tau_j t^j = y_{n+i}, \quad i = k - 1. \tag{4}$$

$$\sum_{j=0}^{k+3} j\tau_j t^{j-1} = f_{n+i}, \quad i = 0, \ldots, k. \tag{5}$$

$$\sum_{j=0}^{k+3} j(j-1)\tau_j t^{j-2} = g_{n+i}, \quad i = k. \tag{6}$$

$$\sum_{j=0}^{k+3} j(j-1)(j-2)\tau_j t^{j-3} = \gamma_{n+k}, \quad i = k. \tag{7}$$

The $(k + 4)$ undetermined coefficients τ_j are obtained by solving Eqs. (3)–(6) and are then substituted into (2). After some algebraic simplification the continuous representation of the third derivative method obtained is given in the form

$$Y(t) = y_{n+k-1} + h\sum_{j=0}^{k} \alpha_j(t) f_{n+j} + h^2 \beta_k(t) g_{n+k} + h^3 \eta_k(t) \gamma_{n+k} \tag{8}$$

where $\alpha_j(t)$, $j = 0, 1, \ldots, k$, $\beta_k(t)$, and $\eta_k(t)$, are continuous coefficients k is the step number, and h is the chosen step-length. We assume that $y_{n+j} = Y(t_n + jh)$ is the numerical approximation to the analytical solution $y(t_{n+j})$, $y'_{n+j} = f(t_{n+j}, y_{n+j})$ is an approximation to $y'(t_{n+j})$, $g_{n+k} = \frac{df}{dt}(t_{n+k}, y(t_{n+k}))$, and $\gamma_{n+k} = \frac{d^2 f}{dt^2}(t_{n+k}, y(t_{n+k}))$.

The same continuous method (7) is then used to generate the main and additional methods which are combined as block method to provide a global solution for (1).

In what follows the block methods for $k = 2(1)4$ are presented by following the process of derivation above and evaluating (7) at $t = (t_n, t_{n+2})$, $t = (t_n, t_{n+1}, t_{n+3})$ and $t = (t_n, t_{n+1}, t_{n+2}, t_{n+4})$ respectively for $k = 2, 3$ and 4 to yield

$$\left.\begin{aligned} y_n &= y_{n+1} - \frac{49h}{160} f_n - \frac{13h}{10} f_{n+1} + \frac{97h}{160} f_{n+2} - \frac{33h^2}{80} g_{n+2} + \frac{23h^3}{240} \gamma_{n+2} \\ y_{n+2} &= y_{n+1} - \frac{h}{160} f_n + \frac{3h}{10} f_{n+1} + \frac{113h}{160} f_{n+2} - \frac{17h^2}{80} g_{n+2} + \frac{7h^3}{240} \gamma_{n+2} \end{aligned}\right\} \tag{9}$$

$$\left.\begin{aligned} y_n &= y_{n+2} - \frac{121h}{405} f_n - \frac{23h}{15} f_{n+1} + \frac{h}{3} f_{n+2} - \frac{203h}{405} f_{n+3} + \frac{10h^2}{27} g_{n+3} - \frac{4h^3}{45} \gamma_{n+3} \\ y_{n+1} &= y_{n+2} + \frac{h}{90} f_n - \frac{61h}{160} f_{n+1} - h f_{n+2} + \frac{533h}{1440} f_{n+3} - \frac{11h^2}{48} g_{n+3} + \frac{11h^3}{240} \gamma_{n+3} \\ y_{n+3} &= y_{n+2} + \frac{h}{810} f_n - \frac{7h}{480} f_{n+1} + \frac{h}{3} f_{n+2} + \frac{8813h}{12960} f_{n+3} - \frac{83h^2}{432} g_{n+3} + \frac{17h^3}{720} \gamma_{n+3} \end{aligned}\right\} \tag{10}$$

$$\left.\begin{aligned} y_n &= y_{n+3} - \frac{2649h}{8960} f_n - \frac{643h}{420} f_{n+1} - \frac{99h}{560} f_{n+2} - \frac{291h}{140} f_{n+3} - \frac{29083h}{26880} f_{n+4} - \frac{317h^2}{448} g_{n+4} + \frac{33h^3}{224} \gamma_{n+4} \\ y_{n+1} &= y_{n+3} + \frac{29h}{3360} f_n - \frac{1021h}{2835} f_{n+1} - \frac{557h}{420} f_{n+2} - \frac{23h}{105} f_{n+3} - \frac{9367h}{90720} f_{n+4} + \frac{125h^2}{1512} g_{n+4} - \frac{5h^3}{252} \gamma_{n+4} \\ y_{n+2} &= y_{n+3} - \frac{59h}{26880} f_n + \frac{101h}{3780} f_{n+1} - \frac{243h}{560} f_{n+2} - \frac{361h}{420} f_{n+3} + \frac{65059h}{241920} f_{n+4} - \frac{629h^2}{4032} g_{n+4} + \frac{19h^3}{672} \gamma_{n+4} \\ y_{n+4} &= y_{n+3} - \frac{11h}{26880} f_n + \frac{47h}{11340} f_{n+1} - \frac{41h}{1680} f_{n+2} + \frac{151h}{420} f_{n+3} + \frac{479833h}{725760} f_{n+4} - \frac{2159h^2}{12096} g_{n+4} + \frac{41h^3}{2016} \gamma_{n+4} \end{aligned}\right\}. \tag{11}$$

3. Analysis of the method

3.1. Order of accuracy

Following Lambert [1] and Fatunla [10] we define the local truncation error associated with the above methods to be the linear difference operator

$$L[y(t); h] = \sum_{j=0}^{k} \varphi_j y(t + jh) - h \sum_{j=0}^{k} \alpha_j y'(t + jh) - h^2 \beta_k y''(t + kh) - h^3 \eta_k y'''(t + kh). \tag{12}$$

Assuming that $y(t)$ is sufficiently differentiable, we can write the terms in (12) as a Taylor series expansion of about the point t to obtain the expression

$$L[y(t); h] = C_0 y(t) + C_1 h y'(t) + C_2 h^2 y''(t) + \cdots, + C_p h^p y^p(t) + \cdots \tag{13}$$

where the constant coefficients C_p, $p = 0, 1, 2, \ldots$ are given as follows:

$$C_0 = \sum_{j=0}^{k} \varphi_j$$

$$C_1 = \sum_{j=1}^{k} j\varphi_j - \sum_{j=0}^{k} \alpha_j$$

$$C_2 = \frac{1}{2!}\left(\sum_{j=1}^{k} j^2 \varphi_j - 2\sum_{j=0}^{k} j\alpha_j\right) - \beta_k$$

Table 1
Orders and error constants for block methods $k = 2, 3$ and 4.

k	Order p	Error constant C_{p+1}
2	(5, 5)	$(-\frac{1}{200}, -\frac{1}{1800})^T$
3	(6, 6, 6)	$(\frac{29}{6300}, -\frac{59}{50400}, -\frac{11}{50400})^T$
4	7, 7, 7, 7	$-\frac{31}{6272}, \frac{1}{1323}, -\frac{23}{56448}, -\frac{89}{846720}$

$$C_3 = \frac{1}{3!}\left(\sum_{j=1}^{k} j^3\varphi_j - 3\sum_{j=0}^{k} j^2\alpha_j\right) - k\beta_k - \eta_k$$

$$C_4 = \frac{1}{4!}\left(\sum_{j=1}^{k} j^4\varphi_j - 4\sum_{j=0}^{k} j^2\alpha_j\right) - \frac{1}{2!}k^2\beta_k - k\eta_k$$

$$\vdots$$

$$C_p = \frac{1}{p!}\left(\sum_{j=1}^{k} j^p\varphi_j - (p-1)\sum_{j=0}^{k} j^{p-1}\alpha_j\right) - \frac{1}{(p-2)!}k^{p-2}\beta_k - \frac{1}{(p-3)!}k^{p-3}\eta_k.$$

According to Henrici [11], the method (2) has order p if

$$L[y(t); h] = O(h^{p+1}), \qquad C_0 = C_1 = \cdots = C_p = 0, \qquad C_{p+1} \neq 0. \tag{14}$$

Therefore, C_{p+1} is the error constant and $C_{p+1}h^{p+1}y^{(p+1)}(t_n)$ the principal local truncation error at the point t_n. It was established from our calculations that the block methods for $k = 2, 3$ and 4 have orders and error constants as displayed in Table 1.

3.2. Stability analysis

In what follows, the k-step third derivative block method can generally be rearranged and rewritten as a matrix finite difference equation of the form

$$A^{(1)}Y_{\omega+1} = A^{(0)}Y_\omega + hB^{(1)}F_{\omega+1} + hB^{(0)}F_\omega + h^2D^{(1)}G_\omega + h^3E^{(1)}R_\omega F_\omega \tag{15}$$

where

$$Y_{\omega+1} = (y_{n+1}, y_{n+2}, y_{n+3}, \ldots, y_{n+k-1}, y_{n+k})^T,$$
$$Y_\omega = (y_{n-k+1}, y_{n-k+2}, y_{n-k+3}, \ldots, y_{n-1}, y_n)^T$$
$$F_{\omega+1} = (f_{n+1}, f_{n+2}, f_{n+3}, \ldots, f_{n+k})^T,$$
$$F_\omega = (f_{n-k+1}, f_{n-k+2}, f_{n-k+3}, \ldots, f_{n-1}, f_n)^T$$
$$G_{\omega+1} = (g_{n+1}, g_{n+2}, g_{n+3}, \ldots, g_{n+k})^T,$$
$$R_{\omega+1} = (\gamma_{n+1}, \gamma_{n+2}, \gamma_{n+3}, \ldots, \gamma_{n+k})^T,$$

for $\omega = 0, \ldots$ and $n = 0, k, \ldots, N-k$.

And the matrices $A^{(1)}$, $A^{(0)}$, $B^{(1)}$, $B^{(0)}$, D^1 and $E^{(1)}$ are k by k matrices whose entries are given by the coefficients of (9)–(11)

3.2.1. Linear stability

The linear stability properties of the newly derived methods are determined by expressing them in the form (15) and applying them to the test problem $y' = \lambda y$, $y'' = \lambda^2 y$, $y''' = \lambda^3 y$, $\lambda < 0$ to yield

$$Y_{\omega+1} = M(z)Y_\omega, \qquad z = \lambda h, \tag{16}$$

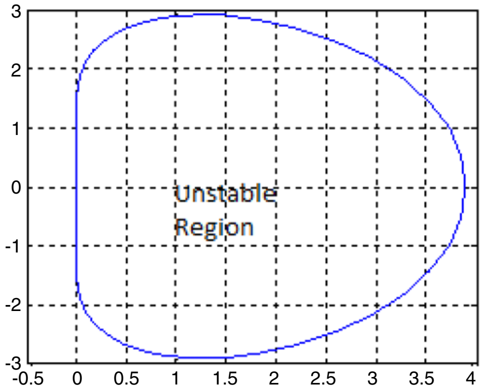

Fig. 1. Region of absolute stability for $k = 2$.

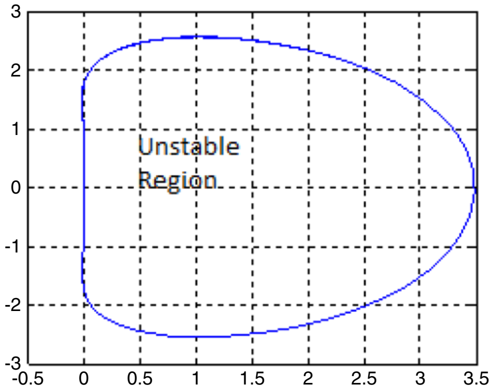

Fig. 2. Region of absolute stability for $k = 3$.

where the amplification matrix $M(z)$ is given by

$$M(z) = -(A^{(1)} - zB^{(1)} - z^2D^1 - z^3E^1)^{-1}(A^{(0)} + zB^0). \tag{17}$$

The matrix $M(z)$ has eigenvalues $\{\zeta_1, \zeta_2, \zeta_3, \ldots, \zeta_k\} = \{0, 0, 0, \ldots, \zeta_k\}$, where the dominant eigenvalue ζ_k is the stability function $R(z) : \mathbb{C} \to \mathbb{C}$ which is a rational function with real coefficients. In particular, taking $k = 2, 3, 4$, we have that

$K = 2$

$$\zeta_2(z) = \frac{1 + 0.6z + 0.1z^2}{1 - 1.4z + 0.9z^2 - 0.3333333z^3 + 0.06666667z^4}$$

$K = 3$

$$\zeta_3(z) = \frac{-1 - z - 0.366667z^2 - 0.05z^3}{-1 + 2z - 1.86667z^2 + 1.05z^3 - 0.375z^4 + 0.075z^5}$$

$K = 4$

$$\zeta_4(z) = \frac{-1 - 1.439z - 0.833z^2 - 0.238z^3 - 0.02857z^4}{-1 + 4.735z - 0.6666z^2 + 3.3809z^3 - 0.9963z^4 + 0.39365z^5 - 0.07619z^6}.$$

The Region of Absolute Stability (RAS) of the methods are plotted using the root locus technique. The RAS for methods $k = 2, 3$, and 4 are shown below. (see Figs. 1–3)

The unstable region is the interior of the curve while the stable region contains the entire left half complex plane. Clearly, the methods are A-stable and also L-stable since the stability function $\zeta_k(z)$ satisfies the additional condition $\lim_{z\to\infty}\zeta_k(z) = 0$.

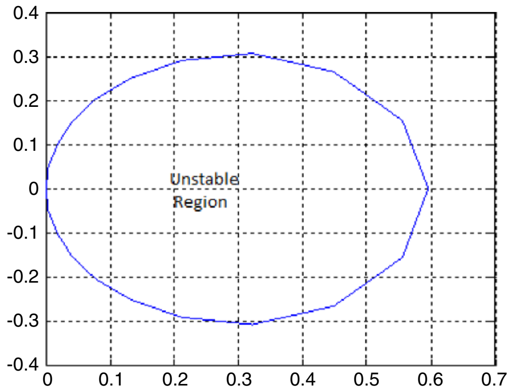

Fig. 3. Region of absolute stability for $k = 4$.

4. Numerical examples

In this section, numerical examples are presented to illustrate the efficiency of the derived third derivative block methods. All absolute errors of the approximate solution are given as $|y - y(x)|$. All computations were carried out using a written code in Matlab 14.0.

Example 4.1. Consider the stiff system

$$y_1' = -y_1 - 15y_2 + 15e^{-t} \quad y_1(0) = 1,$$
$$y_2' = 15y_1 - y_2 - 15e^{-t} \quad y_1(0) = 1.$$

Its Exact solution is $y_1(t) = y_2(t) = e^{-t}$.
This system has eigenvalues of large modulus lying close to the imaginary axis $-115i$. This problem is solved using one of the derived methods and compared with that of $k = 2$ with the numerical solution of 2-step Hojjati SDMM and 3-step EBDF with $h = 0.01$. It is seen that 2-step third derivative block method is superior to the 2-step Hojjati SDMM and 3-step EBDF.

Example 4.2. Consider the Stiffly nonlinear problem which was solved by Vaquero and Vigo-Aguiar [12] and Hojjati et al. [7] in the range $0 \leq t \leq T$

$$y_1' = -(\epsilon^{-1} + 2)y_1 + \epsilon^{-1}y_2; \quad y_1(0) = 1.$$
$$y_2' = y_1 - y_2 - y_2^2; \quad y_2(0) = 1.$$

The smaller ϵ is, the more serious the stiffness of the system. Its exact solution is given by

$$y_1 = y_2^2, \qquad y_2 = e^{-t}.$$

The results for this problem obtained by Vaquero and Vigo-Aguiar [12] using an Exponentially-Fitted Gauss (EF-Gauss-2s) and Gauss-2s methods of order 4 together with that obtained by Hojjati et al. [7] using Second Derivative Multistep Method (SDMM) and Extended Backward Differentiation Formula (EBDF) are displayed in Tables 3 and 4 and compared with the results given by the newly derived CTDBM.
It is seen from Tables 3 and 4 as expected that the CTDBM for $k = 2$ performs better than those in [12] and [7]. Below is the result for the CTDBM for $k = 3, 4$.

Example 4.3. We consider the system of stiff differential equations

$$y_1' = -20y_1 - 0.25y_2 - 19.75y_3; \quad y_1(0) = 1.$$
$$y_2' = 20y_1 - 20.25y_2 + 0.25y_3; \quad y_2(0) = 0.$$
$$y_3' = 20y_1 - 19.75y_2 - 0.25y_3; \quad y_3(0) = -1.$$

Table 2
The absolute error at $t = 5, 10, 15, 20$ for Example 4.1.

t	Error in EBDF ($K = 3$) y_1 y_2	Error in SDMM ($K = 2$) y_1 y_2	Error in CTDBM ($K = 2$) y_1 y_2
5.0	2.37×10^{-12}	6.09×10^{-14}	3.73×10^{-17}
	2.59×10^{-12}	2.24×10^{-14}	9.54×10^{-18}
10	1.81×10^{-14}	7.17×10^{-16}	4.68×10^{-19}
	3.00×10^{-14}	1.12×10^{-16}	2.71×10^{-19}
15	1.01×10^{-16}	6.64×10^{-18}	3.92×10^{-21}
	2.86×10^{-16}	2.86×10^{-19}	2.44×10^{-21}
20	3.36×10^{-19}	5.32×10^{-20}	4.30×10^{-23}
	2.39×10^{-18}	1.31×10^{-20}	4.14×10^{-24}

Table 3
The absolute error at $T = 5$, for Example 4.2.

h	Error in Guass-2s ($p = 4$)	Error in EF-Guass-2s ($p = 4$)	Error in CTDBM ($K = 2, p = 5$)
0.1	5.12×10^{-6}	8.35×10^{-7}	6.78×10^{-10}
0.01	6.45×10^{-12}	4.24×10^{-16}	1.00×10^{-16}

Table 4
The absolute error $h = 0.01$ for Example 4.2.

t	Error in EBDF ($K = 4, p = 5$) y_1 y_2	Error in SDMM ($K = 3, p = 5$) y_1 y_2	Error in CTDBM ($K = 2, p = 5$) y_1 y_2
5.0	3.92×10^{-15}	3.92×10^{-16}	1.00×10^{-16}
	2.70×10^{-13}	3.72×10^{-14}	7.49×10^{-15}
10	3.43×10^{-19}	4.56×10^{-20}	9.11×10^{-21}
	3.61×10^{-15}	5.00×10^{-16}	1.00×10^{-16}
20	1.18×10^{-27}	1.28×10^{-28}	3.74×10^{-29}
	3.30×10^{-19}	4.56×10^{-20}	9.08×10^{-21}

The theoretical solution is given by

$$y_1(t) = \frac{1}{2}(e^{-0.5t} + e^{-20t}(\cos(20t) + \sin(20t)))$$
$$y_2(t) = \frac{1}{2}(e^{-0.5t} - e^{-20t}(\cos(20t) - \sin(20t)))$$
$$y_3(t) = -\frac{1}{2}(e^{-0.5t} + e^{-20t}(\cos(20t) - \sin(20t))).$$

5. Conclusion

A newly derived family of Continuous Third Derivative Block Method has been developed for the solution of stiff systems of ordinary differential equations and used to simultaneously solve (1) directly without the need for starting values or predictors. The efficiency of the CTDBM has been demonstrated on some standard numerical examples. Details of the numerical results are displayed in Tables 2–6.

Table 5
The absolute error for Example 4.2.

h	T	Error in CTBDM ($K=3$) y_1 y_2	Error in CTBDDM ($K=4$) y_1 y_2
0.1	5.0	6.33×10^{-13}	4.63×10^{-14}
		4.73×10^{-12}	3.50×10^{-12}
	10	5.82×10^{-17}	4.06×10^{-18}
		6.36×10^{-13}	4.47×10^{-14}
	15	$3.82.01\times10^{-21}$	2.75×10^{-22}
		6.24×10^{-15}	4.53×10^{-16}
	20	2.31×10^{-25}	1.65×10^{-26}
		5.62×10^{-17}	4.01×10^{-18}
0.01	5.0	7.30×10^{-19}	5.62×10^{-21}
		5.46×10^{-17}	4.18×10^{-19}
	10	6.06×10^{-23}	4.99×10^{-25}
		7.27×10^{-19}	5.50×10^{-21}
	15	4.47×10^{-27}	2.75×10^{-29}
		7.30×10^{-21}	4.53×10^{-23}
	20	2.69×10^{-31}	1.65×10^{-33}
		6.55×10^{-23}	4.01×10^{-25}

Table 6
The absolute error $h=0.01$ for Example 4.3.

t	Error in CTBDM ($K=2$) y_1 y_2 y_3	Error in CTBDM ($K=3$) y_1 y_2 y_3	Error in CTDBM ($K=4$) y_1 y_2 y_3
10	1.16×10^{-16}	4.20×10^{-19}	1.57×10^{-21}
	1.16×10^{-16}	4.20×10^{-19}	1.57×10^{-21}
	1.16×10^{-16}	4.20×10^{-19}	1.57×10^{-21}
20	1.56×10^{-21}	5.65×10^{-20}	2.12×10^{-23}
	1.56×10^{-21}	5.65×10^{-16}	2.12×10^{-23}
	1.56×10^{-21}	5.65×10^{-16}	2.12×10^{-23}
30	1.58×10^{-23}	5.71×10^{-28}	2.14×10^{-25}
	1.58×10^{-23}	5.71×10^{-28}	2.14×10^{-25}
	1.58×10^{-23}	5.71×10^{-20}	2.14×10^{-25}

Acknowledgments

We are grateful to the referees whose useful suggestions greatly improve the quality of this manuscript.

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