

Third Derivative Generalized Backward Differentiation Formulas For Stiff Systems

G. C. Nwachukwu and T. Okor

Department of Mathematics, University of Benin, Benin City, Nigeria.

Abstract

In this paper we present a class of third derivative generalized backward differentiation formulas (TDGBDF) which is based on the linear multistep formulas (LMF). The class of methods developed herein and applied as boundary value methods (BVMs) has good accuracy and stability properties suitable for stiff initial value problems (IVPs) in ordinary differential equations (ODEs). The stability properties of the TDGBDF are discussed. The TDGBDF are $A_{v,k-v}$ -stable and $0_{v,k-v}$ -stable with $(v, k-v)$ -boundary conditions for all values of $k \geq 2$ with order $p = k + 2$ where k is the steplength.

Keywords: Linear Multistep Formulas, Boundary Value Methods, $A_{v,k-v}$ -stable

1. INTRODUCTION

Stiffness exhibited by most differential equations of the form:

$$y' = f(x, y), \quad x \in [t_0, T], \quad y(x_0) = y_0, \tag{1.1}$$

has remained intractable by many ODE methods. Several authors discussed problems of stiffness ([1 - 6]). A potentially good numerical method for the solution of stiff systems of ODEs must have good accuracy and infinite region of absolute stability ([7]). Backward differentiation formulas proposed in [8] and implemented in [9] are famous for their suitability for the integration of stiff differential equations. Methods for stiff ODEs were considered in [5, 10 - 23] and others. In this paper we introduce a new class of TDGBDF with good accuracy and stability properties suitable for stiff differential equations. The paper is organized as follows. In Section 2, we recall the main facts about BVMs. Section 3 is devoted to the derivation and the analysis of the proposed class of methods. The computational aspects for the implementation of the methods are given in Section 4 to demonstrate how the class of methods are applied as BVMs to (1.1) while in Section 5 numerical experiments are carried out to show the efficiency of this class of methods and finally we gave the conclusion of the paper in Section 6.

2. Boundary Value Methods (BVMs)

The numerical solution of the IVP (1.1) is usually obtained by using the k -step LMF

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} \tag{2.1}$$

Where y_n denotes the discrete approximation of the solution $y(x_n)$ at $x = x_n$ and $h = (T - t_0)/N$ and $f_n = f(x_n, y_n)$. If k_1 and k_2 are two integers such that $k_1 + k_2 = k$ and k_1 are the conditions at the initial points and k_2 are given conditions at the final points. Then one may impose the k conditions for the LMF (2.1) by fixing the first $k_1 (\leq k)$ values of the discrete solution, $y_0, y_1, \dots, y_{k_1-1}$ and the last $k_2 = k - k_1$ values, y_{N-k_2+1}, \dots, y_N yielding the discrete method

$$\sum_{i=-k_1}^{k_2} \alpha_{i+k_1} y_{n+i} = h \sum_{i=-k_1}^{k_2} \beta_{i+k_1} f_{n+i}, \quad n = k_1, \dots, N - k_2, \tag{2.2}$$

$y_0, y_1, \dots, y_{k_1-1}, \quad y_{N-k_2+1}, \dots, y_N$ fixed

In this case the given continuous IVP (1.1) is approximated by means of a discrete boundary value problem. The resulting class of methods is referred to as BVMs with (k_1, k_2) -boundary conditions. For $k_1 = k$ and therefore $k_2 = 0$, one has the initial value methods (IVMs). So the class of IVMs is a sub class of BVMs for ODEs based on LMF ([24]).

The continuous problem (1.1) provides only the initial value y_0 . According to [24], to implement (2.2) as a BVM, the $k - 1$ additional values $y_1, \dots, y_{k_1-1}, \quad y_{N-k_2+1}, \dots, y_N$ are obtained by introducing a set of $k - 1$ additional equations which are

Correspondence Author: Nwachukwu G.C., E-mail: grace.nwachukwu@uniben.edu, Phone: +2348056743776

derived by a set of $k_1 - 1$ additional initial methods

$$\sum_{i=0}^k \alpha_i^{(j)} y_i = h \sum_{i=0}^k \beta_i^{(j)} f_i$$

$$j = 1, \dots, k_1 - 1 \tag{2.3}$$

and k_2 final methods

$$\sum_{i=0}^k \alpha_{k-i}^{(j)} y_{N-i} = h \sum_{i=0}^k \beta_{k-i}^{(j)} f_{N-i}$$

$$j = N - k_2 + 1, \dots, N \tag{2.4}$$

The equations (2.2), (2.3) and (2.4) form a composite scheme assumed to be of the same order where (2.3) and (2.4) are the most suitable set of additional methods.

Definition 2.1

Consider a polynomial $p(z)$, such that p is a function of a complex variable z , calculated by the formula:

$$p(z) = \sum_{j=0}^k \alpha_j z^{k-j} = \alpha_0 z^k + \alpha_1 z^{k-1} + \dots + \alpha_k \quad (\alpha_0 \neq 0)$$

The zeros of the polynomial $p(z)$ are denoted by $z_i, i = 1, \dots, k$. If the zeros z_i are simple for all values of i , their multiplicities are equal to one.

The polynomial $p(z)$ is called the Schur polynomial if for all values of $i = 1, \dots, k$ the condition $|z_i| < 1$ is satisfied.

The polynomial $p(z)$ is called the Von Neumann polynomial if for all values of $i = 1, \dots, k$ the condition $|z_i| \leq 1$ is satisfied ([25]).

Definition 2.2 ([5])

A polynomial $p(z)$ of degree $k = k_1 + k_2$ is a $S_{k_1 k_2}$ -polynomial if its roots are such that $|z_1| \leq |z_2| \leq \dots \leq |z_{k_1}| < 1 < |z_{k_1+1}| \leq \dots \leq |z_k|$ and it is a $N_{k_1 k_2}$ -polynomial if $|z_1| \leq |z_2| \leq \dots \leq |z_{k_1}| \leq 1 < |z_{k_1+1}| \leq \dots \leq |z_k|$ being simple the roots of unit modulus.

Observe that for $k_1 = k$ and $k_2 = 0$ a $N_{k_1 k_2}$ -polynomial reduces to a Von Neumann polynomial and a $S_{k_1 k_2}$ -polynomial reduces to a Schur polynomial.

Let $\rho(z) = \sum_{j=0}^k \alpha_j z^j$ and $\sigma(z) = \sum_{j=0}^k \beta_j z^j$ denote the two characteristic polynomials associated with the LMM (2.2).

Thus $\prod(z, q) = \rho(z) - q\sigma(z), q = h\lambda$, is the stability polynomial when (2.2) is applied on $y' = \lambda y, Re(\lambda) < 0$. Then we have the following definitions, see [5]:

Definition 2.3

A BVM with (k_1, k_2) -boundary conditions is $O_{k_1 k_2}$ -stable if $\rho(z)$ is a $N_{k_1 k_2}$ -polynomial.

Observe that $O_{k_1 k_2}$ -stability reduces to the usual zero-stability from Definition 2.2 for LMM when $k_1 = k$ and $k_2 = 0$.

Definition 2.4

(a) For a given $q \in \mathbb{C}$, a BVM with (k_1, k_2) -boundary conditions is (k_1, k_2) -absolutely stable if $\prod(z, q)$ is a $S_{k_1 k_2}$ -polynomial. Again, (k_1, k_2) -absolute stability reduces to the usual notion of absolute stability when $k_1 = k$ and $k_2 = 0$ for LMM.

(b) Similarly, one defines the region of (k_1, k_2) -absolute stability of the method as

$$D_{k_1 k_2} = \{q \in \mathbb{C} : \prod(z, q) \text{ is a } S_{k_1 k_2} \text{-polynomial}\}. \text{ Here } \prod(z, q) \text{ is a polynomial of type } (k_1, 0, k_2)$$

(c) A BVM with (k_1, k_2) -boundary conditions is said to be $A_{k_1 k_2}$ -stable if $\mathbb{C}^- \subseteq D_{k_1 k_2}$.

3. Derivation And Analysis Of The Third Derivative Generalized Backward Differentiation Formulae (TDGBDF)

The third derivative backward differentiation formula (TDBDF)

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k f_{n+k} + h^2 \gamma_k f'_{n+k} + h^3 \delta_k f''_{n+k} \tag{3.1}$$

where $f_{n+k}, f'_{n+k}, f''_{n+k}$ are the first, second and third derivatives functions respectively, is A -stable for step number $k = 2(1)4$ are $A(\alpha)$ -stable for $k = 1, k = 5(1)9$ and unstable for $k \geq 10$ ([21]).

Following the idea of [5, 14] we rewrite the TDBDF (3.1) as

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_i f_{n+i} + h^2 \gamma_i f'_{n+i} + h^3 \delta_i f''_{n+i} \tag{3.2}$$

where $i = 0, 1, 2, \dots, k$ and δ_k has been normalized to 1. For $i = k$ the TDBDF (3.2) is used as IVM. But for $i \neq k$ it is used as BVM and we gain the liberty of choosing the values of i for which method (3.2) has the most suitable stability properties. Specifically for the choice of $i = v$ such that:

$$v = \begin{cases} \frac{k+2}{2} & \text{for even } k \\ \frac{k+3}{2} & \text{for odd } k \end{cases} \quad (3.3)$$

The formula (3.2) becomes

$$\sum_{j=0}^k \alpha_j y_{n+j} = h\beta_v f_{n+v} + h^2 \gamma_v f'_{n+v} + h^3 f''_{n+v} \quad (3.4)$$

where α_j, β_v and γ_v are parameters to be determined by imposing the formula (3.4) to reach its highest possible order which is $k + 2$. The class of methods (3.4) which is $O_{v,k-v}$ -stable and $A_{v,k-v}$ -stable for all values of $k \geq 2$ is called the TDGBDF and must be used with $(v, k - v)$ boundary conditions ([5, 14, 24, 26]). In order to obtain the parameters of the class of methods (3.4) we rewrite (3.4) as :

$$\sum_{j=0}^k \alpha_j y(x + jh) = h\beta_v y'(x + vh) + h^2 \gamma_v y''(x + vh) + h^3 y'''(x + vh) \quad (3.5)$$

where $y_{n+j} = y(x + jh), f_{n+v} = y'(x + vh), f'_{n+v} = y''(x + vh)$ and $f''_{n+v} = y'''(x + vh)$. Expanding (3.5) in Taylor's series and applying the method of undetermined coefficients yields a system of linear equations from which the coefficients α_j, β_v and γ_v are determined as the solutions of the resulting system of linear equations ([27, 28]). The coefficients of (3.4) are reported in table 1.

According to [29] in order to analyze the stability of the specific method, we applied the test problems:

$$y' = \lambda y, \quad y'' = \lambda^2 y, \quad y''' = \lambda^3 y$$

to the class of methods (3.4) to yield the characteristic equation:

$$\sum_{j=0}^k \alpha_j z^j - (q\beta_v + q^2\gamma_v + q^3)z^v = 0, \quad q = \lambda h, \quad q \in \mathbb{C} \quad (3.6)$$

where v is defined as in (3.3). Inserting $z = e^{i\theta}$, (3.6) gives us three roots describing the stability regions for the odd and even values of k given in figures 1 and 2 respectively.

In accordance with [2, 30] we define the local truncation error associated with (3.4) as the linear difference operator,

$$L(y(x); h) = \sum_{j=0}^k \alpha_j y(x + jh) - h\beta_v y'(x + vh) - h^2 \gamma_v y''(x + vh) - h^3 y'''(x + vh)$$

Assuming that $y(x)$ is sufficiently differentiable, by Taylor's series expansion of $y(x + jh), y'(x + vh), y''(x + vh)$ and $y'''(x + vh)$ the $L(y(x); h)$ is obtained in the form

$$L(y(x); h) = C_0 y(x) + C_1 h y'(x) + C_2 h^2 y''(x) + \dots + C_q h^q y^{(q)}(x) + \dots \quad (3.7)$$

$$\left. \begin{aligned} C_0 &= \sum_{j=0}^k \alpha_j \\ C_1 &= \left[\sum_{j=0}^k j \alpha_j - \beta_v \right] \\ C_2 &= \left[\sum_{j=0}^k \frac{j^2 \alpha_j}{2!} - v\beta_v - \gamma_v \right] \\ &\vdots \\ C_q &= \left[\sum_{j=0}^k \frac{j^q \alpha_j}{q!} - \frac{\beta_v v^{q-1}}{(q-1)!} - \frac{\gamma_v v^{q-2}}{(q-2)!} - \frac{v^{q-3}}{(q-3)!} \right] \end{aligned} \right\} \quad (3.8)$$

The TDGBDF (3.4) is said to be of order p if

$$C_0 = C_1 = C_2 = \dots = C_p = 0, C_{p+1} \neq 0$$

Therefore, C_{p+1} is the error constant (EC) and $C_{p+1} h^{p+1} y^{(p+1)}(x)$ is the principal local truncation error at the point x . The error constant and the order of the TDGBDF (3.4) are given in Table 1.

Table 1 Coefficient List of the TDGBDF for $k = 1, 2, \dots, 10$

k	v	p	α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	β_v	γ_v	C_{p+1}
1	2	3	$-\frac{6}{7}$	$\frac{6}{7}$										$\frac{6}{7}$	$-\frac{9}{7}$	$\frac{15}{28}$
2	2	4	$\frac{3}{4}$	-12	$\frac{45}{4}$									$\frac{21}{2}$	$-\frac{9}{2}$	$\frac{1}{10}$
3	3	5	$-\frac{2}{9}$	$\frac{9}{4}$	-18	$\frac{575}{36}$								$\frac{85}{6}$	$-\frac{11}{2}$	$\frac{1}{20}$
4	3	6	$-\frac{1}{18}$	$\frac{3}{4}$	-9	$\frac{245}{36}$	$\frac{3}{2}$							$\frac{55}{6}$	$-\frac{5}{2}$	$-\frac{1}{140}$
5	4	7	$\frac{3}{160}$	$-\frac{2}{9}$	$\frac{3}{2}$	-12	$\frac{2737}{288}$	$\frac{6}{5}$						$\frac{259}{24}$	$-\frac{13}{4}$	$-\frac{1}{280}$
6	4	8	$\frac{1}{160}$	$-\frac{4}{45}$	$\frac{3}{4}$	-8	$\frac{1435}{288}$	$\frac{12}{5}$	$-\frac{1}{20}$					$\frac{217}{24}$	$-\frac{7}{4}$	$\frac{1}{1260}$
7	5	9	$-\frac{2}{875}$	$\frac{1}{32}$	$-\frac{2}{9}$	$\frac{5}{4}$	-10	$\frac{251243}{36000}$	2	$-\frac{1}{28}$				$\frac{5989}{600}$	$-\frac{47}{20}$	$\frac{1}{2520}$
8	5	10	$-\frac{3}{3500}$	$\frac{3}{224}$	$-\frac{1}{9}$	$\frac{3}{4}$	$-\frac{15}{2}$	$\frac{15807}{4000}$	3	$-\frac{3}{28}$	$\frac{1}{252}$			$\frac{5449}{600}$	$-\frac{27}{20}$	$-\frac{1}{9240}$
9	6	11	$\frac{1}{3024}$	$-\frac{9}{1750}$	$\frac{9}{224}$	$-\frac{2}{9}$	$\frac{9}{8}$	-9	$\frac{200453}{36000}$	$\frac{18}{7}$	$-\frac{9}{112}$	$\frac{1}{378}$		$\frac{5819}{600}$	$-\frac{37}{20}$	$-\frac{1}{18480}$
10	6	12	$\frac{1}{7560}$	$-\frac{2}{875}$	$\frac{9}{448}$	$-\frac{8}{63}$	$\frac{3}{4}$	$-\frac{36}{5}$	$\frac{59059}{18000}$	$\frac{24}{7}$	$-\frac{9}{56}$	$\frac{2}{189}$	$-\frac{1}{2240}$	$\frac{5489}{600}$	$-\frac{11}{10}$	$\frac{1}{60060}$

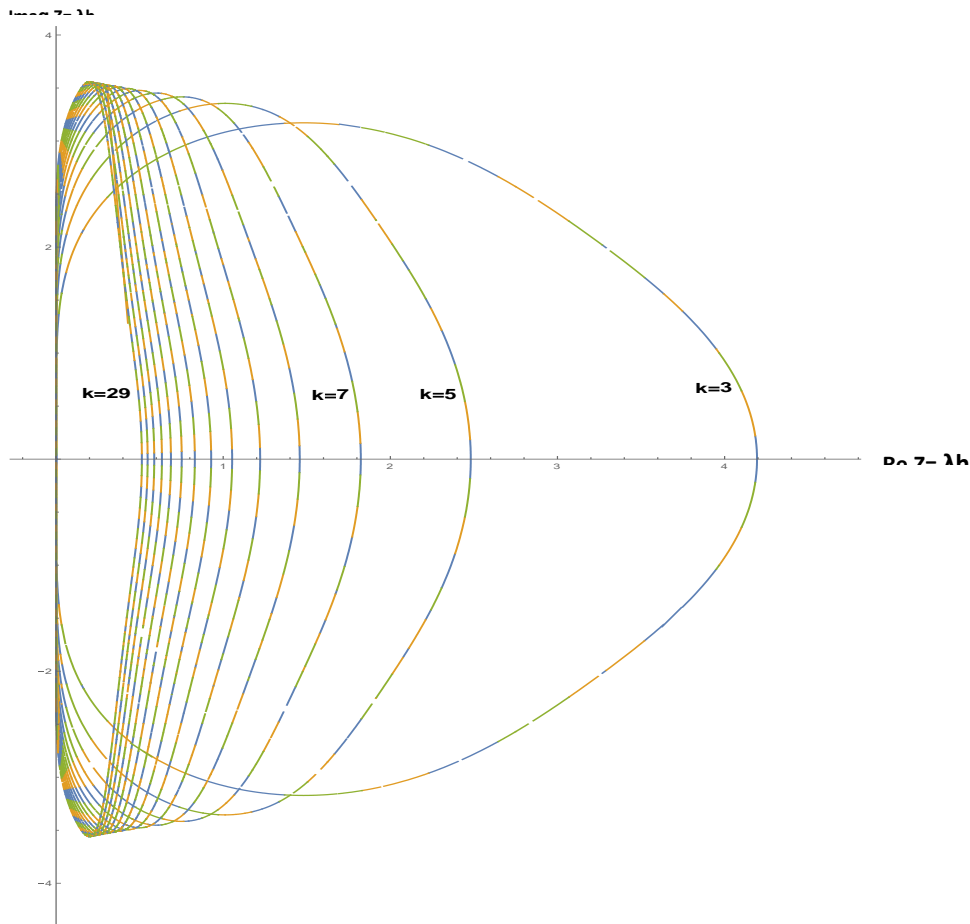


Figure 1: Stability regions of TDGBDF for k odd ($k = 3, 5, \dots, 29$)

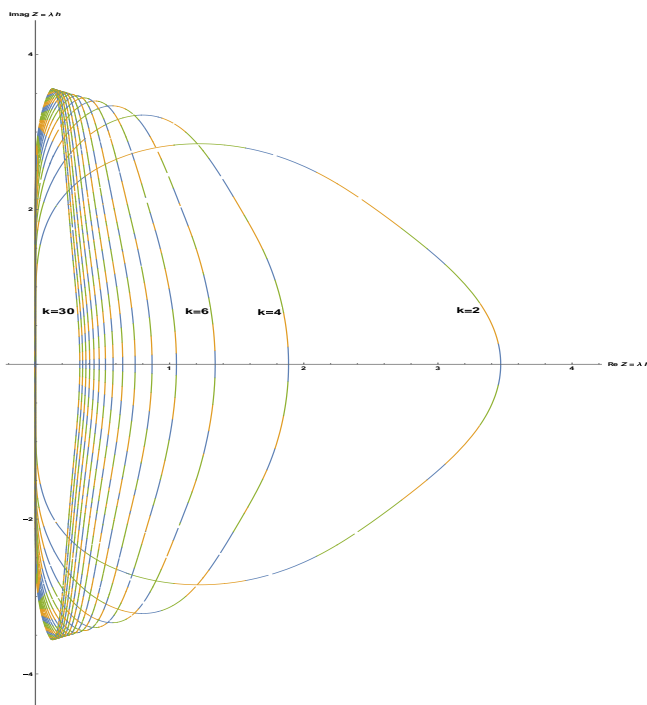


Figure 2: Stability regions of TDGBDF for k even ($k = 2, 4, \dots, 30$)

4. IMPLEMENTATION PROCEDURE

In this section, the implementation procedure for the proposed class of methods (of order 6 and 7) as BVMs in the sense of [5, 14] is given. The class of methods (3.4) requires $(v - 1, k - v)$ initial and final additional methods for its implementation (Note: $v - 1$ initial methods since y_0 is already provided by the problem to be solved). The methods (3.4) are used alongside the following additional initial methods which we defined generally as:

$$\sum_{j=0}^k \alpha_j^* y_{n+j}^* = h\beta_i f_i + h^2 \gamma_i f_i' + h^3 f_i''; \quad i = 1, 2, \dots, v-1 \quad (4.1)$$

And final methods given generally as:

$$\sum_{j=0}^k \alpha_j^* y_{n+j}^* = h\beta_i f_i + h^2 \gamma_i f_i' + h^3 f_i''; \quad i = v+1, \dots, N \quad (4.2)$$

The TDGBDF of order 6 is $A_{3,1}$ -stable and $0_{3,1}$ -stable with (3,1) boundary conditions. It therefore requires 2 initial methods and 1 final method (where $k = 4$ and $v = 3$) for its implementation. The TDGBDF of order 6 is given as:

$$-\frac{1}{18}y_n + \frac{3}{4}y_{n+1} - 9y_{n+2} + \frac{245}{36}y_{n+3} + \frac{3}{2}y_{n+4} = \frac{55}{6}hf_{n+3} - \frac{5}{2}h^2f_{n+3}' + h^3f_{n+3}'' \quad (4.3)$$

We rewrite the main method (TDGBDF of order 6) as ([5, 14]):

$$-\frac{1}{18}y_{n-3} + \frac{3}{4}y_{n-2} - 9y_{n-1} + \frac{245}{36}y_n + \frac{3}{2}y_{n+1} = \frac{55}{6}hf_n - \frac{5}{2}h^2f_n' + h^3f_n'' \quad (4.4)$$

$$n = 3, \dots, N-1$$

We use (4.4) together with the following initial methods ($n = 0$) obtained from (4.1):

$$\text{first initial method: } -\frac{3}{2}y_0 - \frac{245}{36}y_1 + 9y_2 - \frac{3}{4}y_3 + \frac{1}{18}y_4 = \frac{55}{6}hf_1 + \frac{5}{2}h^2f_1' + h^3f_1'' \quad (4.5)$$

$$\text{second initial method: } \frac{1}{8}y_0 - 4y_1 + 4y_3 - \frac{1}{8}y_4 = \frac{15}{2}hf_2 + h^3f_2'' \quad (4.6)$$

and final method obtained from (4.2) given below:

$$\frac{3}{32}y_{N-4} - \frac{8}{9}y_{N-3} + \frac{9}{2}y_{N-2} - 24y_{N-1} + \frac{5845}{288}y_N = \frac{415}{24}hf_N - \frac{25}{4}h^2f_N' + h^3f_N'' \quad (4.7)$$

The TDGBDF of order 7 is $A_{4,1}$ -stable and $0_{4,1}$ -stable with (4,1) boundary conditions. It requires 3 initial methods and 1 final method (where $k = 5$ and $v = 4$). The TDGBDF of order 7 is given as:

$$\begin{aligned} & \frac{3}{160}y_n - \frac{2}{9}y_{n+1} + \frac{3}{2}y_{n+2} - 12y_{n+3} + \frac{2737}{288}y_{n+4} + \frac{6}{5}y_{n+5} \\ & = \frac{259}{24}hf_{n+4} - \frac{13}{4}h^2f_{n+4}' + h^3f_{n+4}'' \end{aligned} \quad (4.8)$$

As before we write the main method (TDGBDF of order 7) as:

$$\begin{aligned} & \frac{3}{160}y_{n-4} - \frac{2}{9}y_{n-3} + \frac{3}{2}y_{n-2} - 12y_{n-1} + \frac{2737}{288}y_n + \frac{6}{5}y_{n+1} \\ & = \frac{259}{24}hf_n - \frac{13}{4}h^2f_n' + h^3f_n'' \end{aligned} \quad (4.9)$$

$$n = 4, \dots, N-1$$

The method (4.9) is used together with the following initial methods ($n = 0$) obtained from (4.1)

$$\text{first: } -\frac{6}{5}y_0 - \frac{2737}{288}y_1 + 12y_2 - \frac{3}{2}y_3 + \frac{2}{9}y_4 - \frac{3}{160}y_5 = \frac{259}{24}hf_1 + \frac{13}{4}h^2f_1' + h^3f_1'' \quad (4.10)$$

$$\text{2nd: } \frac{3}{40}y_0 - 3y_1 - \frac{49}{18}y_2 + 6y_3 - \frac{3}{8}y_4 + \frac{1}{45}y_5 = \frac{49}{6}hf_2 + h^2f_2' + h^3f_2'' \quad (4.11)$$

$$\text{3rd: } -\frac{1}{45}y_0 + \frac{3}{8}y_1 - 6y_2 + \frac{49}{18}y_3 + 3y_4 - \frac{3}{40}y_5 = \frac{49}{6}hf_3 - h^2f_3' + h^3f_3'' \quad (4.12)$$

And the final method given below is obtained from (4.2):

$$\begin{aligned}
 & -\frac{6}{125}y_{N-5} + \frac{15}{32}y_{N-4} - \frac{20}{9}y_{N-3} + \frac{15}{2}y_{N-2} - 30y_{N-1} + \frac{874853}{36000}y_N \\
 & = \frac{12019}{600}hf_N - \frac{137}{20}h^2f'_N + h^3f''_N
 \end{aligned} \tag{4.13}$$

The methods are implemented as BVMs efficiently by combining the main methods and the additional methods as simultaneous numerical integrators for IVPs and BVPs. In particular, for linear problems, we can solve (1.1) directly from the start with Gaussian elimination partial pivoting. For nonlinear problems, we can use a modified Newton-Raphson method. In each case, the main method and the additional methods are combined as BVMs to give a single matrix of finite difference equations which simultaneously provides the values of the solution and the first derivatives generated by the sequences $\{y_n\}, \{y'_n\}, n = 0, \dots, N$, where the single block matrix equation is solved while adjusting for boundary conditions ([31]).

4.1 IMPLEMENTATION (NUMERICAL EXPERIMENT) OF TDGBDF (4.3) AND (4.8)

The following stiff problems are considered to examine the accuracy of the methods of order $p=6$ (4.3) and 7 (4.8) implemented as block methods.

Problem 1: Test Problem ([5])

$$y' = -\lambda y \quad y(x_0) = y_0, \lambda = 1, 100$$

The exact solution is $y = e^{-\lambda x}$

Problem 2: Singularly Perturbed Problem ([29])

$$y'_1 = -(2 + 10^4)y_1 + 10^4y_2^2, \quad y'_2 = y_1 - y_2 - y_2^2$$

$$y_1(0) = 1, \quad y_2(0) = 1$$

The exact solution is $y_1 = e^{-2x}$, $y_2 = e^{-x}$

Problem 3: Van der Pol equations ([29])(nonlinear problem)

$$y'_1 = y_2, \quad y'_2 = -y_1 + 10y_2(1 - y_1^2)$$

$$y_1(0) = 2, \quad y_2(0) = 0$$

Problem 4: Robertson's equation ([29])(nonlinear problem)

$$y'_1 = -0.04y_1 + 10^4y_2y_3, \quad y'_2 = 0.04y_1 - 3 * 10^7y_2^2 - 10^4y_2y_3, \quad y'_3 = 3 * 10^7y_2^2$$

$$y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0.$$

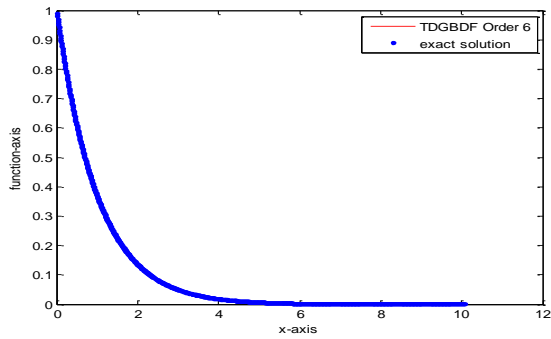


Figure 3A Numerical results for Problem 1 using Method (4.3) $\lambda = 1, h = 0.01$

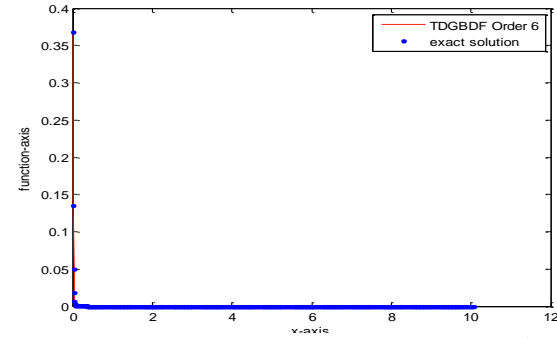


Figure 3B Numerical results for Problem 1 using Method (4.3) $\lambda = 100, h = 0.01$

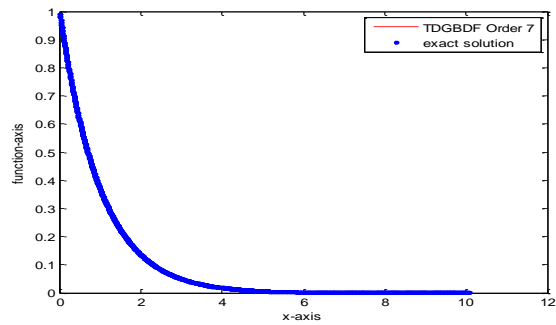


Figure 3C Numerical results for Problem 1 using Method (4.8) $\lambda = 1, h = 0.01$

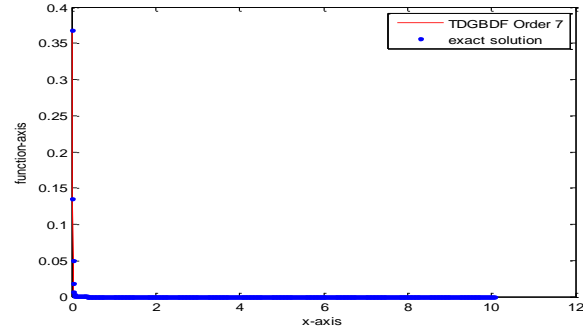


Figure 3D Numerical results for Problem 1 using Method (4.8) $\lambda = 100, h = 0.01$

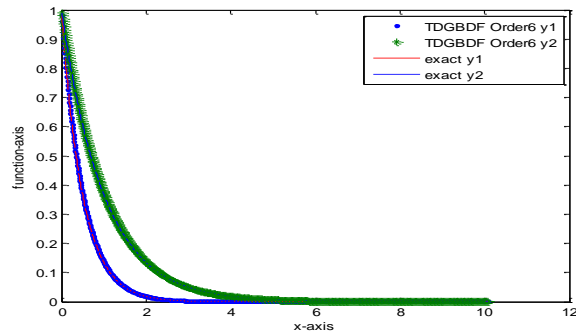


Figure 4A Numerical results for Problem 2 using Method (4.3) $h = 0.01$

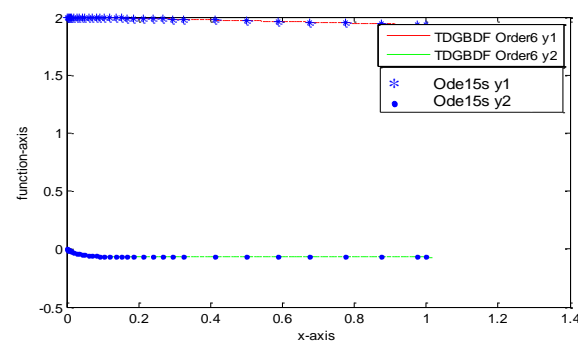


Figure 5A Numerical results for Problem 3 using Method (4.3) $h = 0.001$

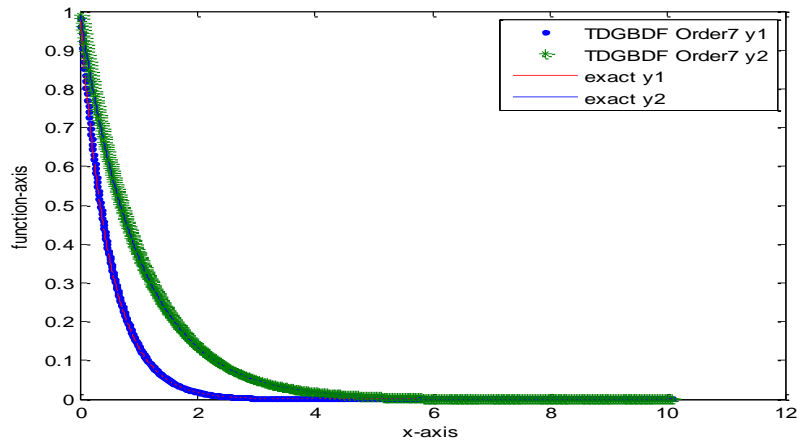


Figure 4B Numerical results for Problem 2 using Method (4.8) $h = 0.01$

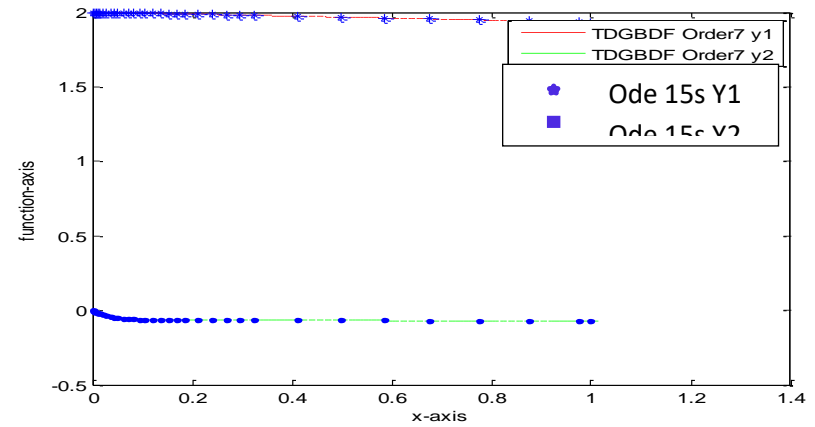


Figure 5B Numerical results for Problem 3 using Method (4.8) $h = 0.001$

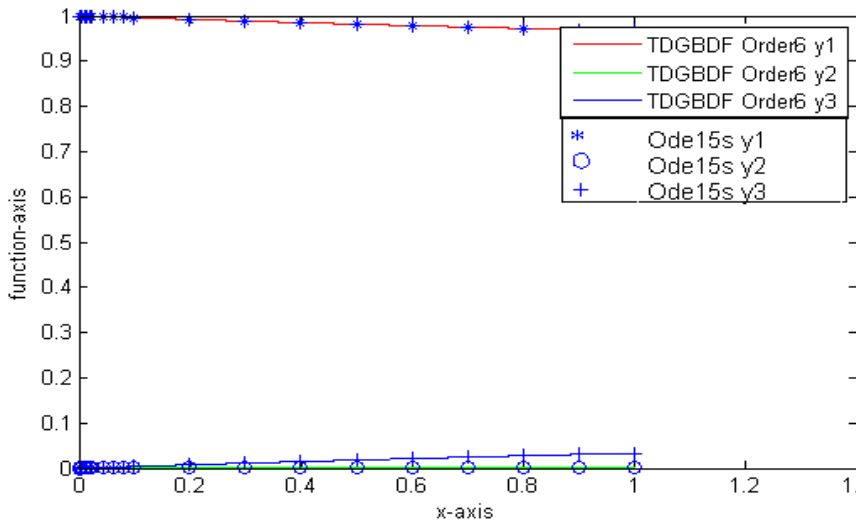


Figure 6A Numerical results for Problem 4 using Method (4.3) $h = 0.001$

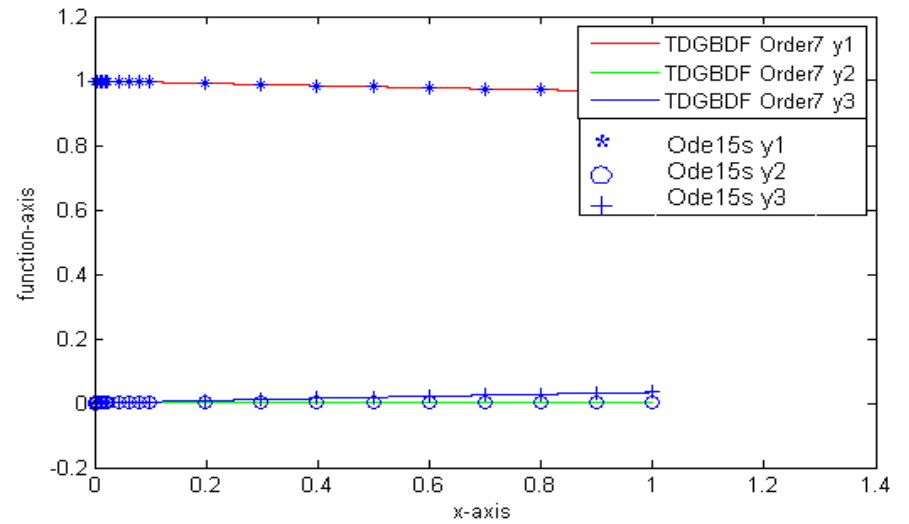


Figure 6B Numerical results for Problem 4 using Method (4.8) $h = 0.001$

TABLE 2A Absolute Error in Problem 1, $h = 0.01$, $\lambda = 100$

x	Error in TDGBDF(4.3) $ y(x_n) - y_n $	Error in TDGBDF(4.8) $ y(x_n) - y_n $
1.0	2.415796612301085e-47	5.494524173111787e-48
2.0	9.590247540521880e-89	2.154118286243749e-89
3.0	1.010926307170304e-133	2.239941880438817e-134
4.0	2.746354900394213e-175	6.008555881761614e-176
5.0	2.400256887600033e-220	5.179272410583249e-221
6.0	5.900748292865801e-262	1.257015286451657e-262
7.0	4.803340357006191e-307	1.009007887963912e-307
8.0	0.000000000000000000	0.000000000000000000
9.0	0.000000000000000000	0.000000000000000000
10.0	0.000000000000000000	0.000000000000000000

TABLE 2B Absolute Error in Problem 1, $h = 0.01$, $\lambda = 1$

x	Error in TDGBDF(4.3) $ y(x_n) - y_n $	Error in TDGBDF(4.8) $ y(x_n) - y_n $
1.0	4.440892098500626e-16	1.609823385706477e-15
2.0	4.996003610813204e-16	4.718447854656915e-16
3.0	3.261280134836397e-16	4.024558464266193e-16
4.0	1.526556658859590e-16	1.040834085586084e-17
5.0	9.280770596475918e-17	9.540979117872439e-18
6.0	4.206704429243757e-17	6.938893903907228e-18
7.0	1.658829323902822e-17	3.903127820947816e-18
8.0	7.96885967768458e-18	1.843143693225358e-18
9.0	3.022213555803344e-18	2.846030702774449e-19
10.0	1.131636017531745e-18	1.355252715606881e-20

TABLE 3A Absolute Error in Problem 2, $h = 0.01$

Errorin TDGBDF (4.3), $ y(x_n) - y_n $		
x	Error y_1	Error y_2
1.0	1.840463059732400e-10	2.638990692638288e-10
2.0	2.729638043375005e-11	1.010463102080195e-10
3.0	3.416046959192620e-12	3.571543755187534e-11
4.0	5.009221119497975e-13	1.367520333084293e-11
5.0	6.258246687800700e-14	4.833577982310544e-12
6.0	9.175104083338891e-15	1.850751323029254e-12
7.0	1.146249982849842e-15	6.541577175778190e-13
8.0	1.680476971405580e-16	2.504715727359719e-13
9.0	2.099441635557973e-17	8.853112470549873e-14
10.0	3.077922929287871e-18	3.389787907835673e-14

TABLE 3B Absolute Error in Problem 2, $h = 0.01$

Errorin TDGBDF (4.8), $ y(x_n) - y_n $		
x	Error y_1	Error y_2
1.0	1.772000601807378e-10	2.550769595544011e-10
2.0	2.512047514446891e-11	9.573458692457848e-11
3.0	3.541552034275197e-12	3.592972447341580e-11
4.0	4.989202952686289e-13	1.348481395990753e-11
5.0	6.109777397553251e-14	4.718898015398931e-12
6.0	8.606149511569336e-15	1.771054223415058e-12
7.0	1.053875957754077e-15	6.197570668470265e-13
8.0	1.484485458811755e-16	2.326036498828676e-13
9.0	2.091033510067494e-17	8.729919998701208e-14
10.0	2.945455330861485e-18	3.276500978085378e-14

Table 4A Errors in Problem 3 using the modulus of the solution of the TDGBDF (4.3) minus the solution of Ode15s, $h = 0.001$. Error $y_i = |y_{i(4.3)} - y_{iOde15s}|$, $i = 1,2$

x	Error y_1	Error y_2
1.0	1.215588347003305e-5	7.136742510016614e-7
5.0	1.388622549969298e-4	5.210835873001307e-6
10.0	2.329715397750842e-4	1.367511946799571e-5
15.0	6.814405109059063e-4	7.564282396299582e-5
20.0	1.923382861019896e-4	6.458919457996704e-6

Table 4B Errors in Problem3 using the modulus of the solution of the TDGBDF (4.8) minus the solution of Ode15s, $h = 0.001$. Error $y_i = |y_{i(4.8)} - y_{iOde15s}|$, $i = 1,2$

x	Error y_1	Error y_2
1.0	1.201686902208010e-5	7.049919770046875e-7
5.0	1.386622152419470e-4	5.238733189000255e-6
10.0	2.331138582791770e-4	1.368338897500543e-5
15.0	6.812137981488942e-4	7.560609076999458e-5
20.0	1.921876518860000e-4	6.449612969000595e-6

Table 5A Errors in Problem 4 using the modulus of the solution of the TDGBDF (4.3) minus the solution of Ode15s, $h = 0.0001$. $\text{Error}y_i = |y_{i(4.3)} - y_{i\text{ode15s}}|$, $i = 1,2,3$

x	Error y_1	Error y_2	Error y_3
1.0	4.419958079537878e-7	7.072967809584971e-11	4.420709879965346e-7
3.0	3.911872170969666e-6	4.932710674992948e-10	3.912369955005879e-6
5.0	4.195654775940305e-6	8.502353418992010e-10	4.196500206998799e-6
7.0	4.281267487094009e-5	4.030955670896721e-9	4.281671028499856e-5
10.0	7.192481450302157e-5	5.640571071999809e-9	7.193045938400089e-5

Table 5B Errors in Problem 4 using the modulus of the solution of the TDGBDF (4.8) minus the solution of Ode15s, $h = 0.0001$. $\text{Error}y_i = |y_{i(4.8)} - y_{i\text{ode15s}}|$, $i = 1,2,3$

x	Error y_1	Error y_2	Error y_3
1.0	4.419921140197403e-7	7.072920270030213e-11	4.420680979957958e-7
3.0	3.911869656980649e-6	4.932708290967896e-10	3.912368173000780e-6
5.0	4.195656818972715e-6	8.502354907025610e-10	4.196501482991999e-6
7.0	5.106982184899245e-5	4.797582577797867e-9	5.107462476097724e-5
10.0	7.192481282003449e-5	5.640571001499562e-9	7.193045868697512e-5

$|y(x_n) - y_n|$ in Tables 2A, 2B, 3A and 3B denote the absolute error. The numerical results in figures 3A, 3B, 3C and 3D for problem 1 and figures 4A and 4B for problem 2 show that the TDGBDF is indistinguishable from the exact solutions. From figures 5A, 5B, 6A and 6B it can be seen that the proposed class of methods is very comparable with the Ode15s. As expected the method of order 7 ($k = 5$) performs better than the method of order 6 ($k = 4$), see Tables 2A, 2B, 3A, 3B, 4A, 4B, 5A and 5B.

7. CONCLUSION

The third derivative generalized backward differentiation formulas (TDGBDF) were developed using the Taylor's series and method of undetermined coefficients. This class of methods (TDGBDF) is $A_{v,k-v}$ -stable and $0_{v,k-v}$ -stable with $(v, k - v)$ -boundary conditions for all values of $k \geq 2$ with order $p = k + 2$. The new methods are well suited for the solution of stiff IVPs in ODEs

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