Second Derivative Generalized Backward Differentiation Formulae for Solving Stiff Problems

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Abstract—**Second derivative generalized backward differentiation formulae (SDGBDF) are developed herein and applied as boundary value methods (BVMs) to solve stiff initial value problems (IVPs) in ordinary differential equations (ODEs). The order, error constant, zero stability and the region of absolute stability for the SDGBDF are discussed. The methods are $A_{v,k-v}$-stable and $0_{v,k-v}$-stable with (v,k-v)-boundary conditions for values of the steplength $k \geq 1$, $v < k$ with order $p = k + 1$.**

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

AMS subject classification: 65L04, 65L05

1 Introduction

The mathematical modeling in science and engineering problems often leads to systems of ordinary differential equations (ODEs) and many of these problems appear to be stiff. A potentially good numerical method for the solution of stiff systems of ODEs must have good accuracy and some reasonably wide region of absolute stability, see [23]. It is on this ground A-stable (stiffly-stable) methods are required.

Consider the initial value problem (IVP)

$$y' = f(x, y),\ x \in [t_0, T],\ y(x_0) = y_0 \qquad (1)$$

Definition 1. *(cf: Lambert [37]). The linear system*

$$y' = Ay + \phi(x), \qquad y(a) = \eta, \qquad a \leq x \leq b \qquad (2)$$

where

$$y = (y_1, y_2 \ldots, y_s) \ \ and \ \ \eta = (\eta_1, \eta_2, \ldots, \eta_s)$$

is said to be stiff if

(i) $Re(\lambda_i) < 0, \quad i = 1, 2, \ldots, s$

(ii)$Max|Re(\lambda_i)| >> Min|Re(\lambda_i)|$

where λ_i *are the eigenvalues of* $s \times s$ *matrix* A*, and the stiff ratio is* $\frac{Max|Re(\lambda_i)|}{Min|Re(\lambda_i)|}$.

Definition 2. *([23]). A numerical integrator is said to be A-stable if its region of absolute stability* R *incorporates the entire left half of the complex plane denoted* $\mathbb{C}$*, i.e.,*

$$R = \{z \in \mathbb{C} | Re(z) \leq 0\}. \qquad (3)$$

Backward differentiation formulae (BDF)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h f_{n+k} \qquad (4)$$

are among the first most popular numerical methods to be proposed for stiff initial value problems (IVPs), see [22, 29]. These methods are found to be A-stable up to order $p = 2$ with order $p = k$ and $A(\alpha) - stable$ for $k = 3(1)6$. In [19] is introduced a class of extended backward differentiation formulae (EBDF)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_k f_{n+k} + h\beta_{k+1} f_{n+k+1} \qquad (5)$$

which has some advantage over the usual BDF. It is found to be A-stable for $k = 1(1)3$ and $A(\alpha) - stable$ for $k = 4(1)8$ with order $p = k + 1$. The modified extended backward differentiation formulae (MEBDF) by [21] is

$$\begin{cases} y_{n+k} - h(\beta_k - v_k) f_{n+k} \\ = -\sum_{j=0}^{k-1} \alpha_j y_{n+j} + h v_k f_{n+k} + h\beta_{k+1} f_{n+k+1} \end{cases} \qquad (6)$$

where the choice of v_k can be defined to maximize in some way the region of absolute stability of (6). The MEBDF is A-stable for $k = 1(1)3$ and $A(\alpha) - stable$ for $k = 4(1)8$ with order $p = k + 1$. The second derivative extended backward differentiation formulae (SDEBDF) by [20] are of two classes in predictor-corrector pair. They are A-stable for $k = 1(1)3$ and $A(\alpha) - stable$ for $k = 4(1)8$ with order $p = k + 2$ and $p \geq k + 3$ for class 1 and $p = k + 3$ for class 2. Other authors such as [34, 26, 42, 5] have also presented some modifications of the BDF. That of [8] and [9] considered the BDF (4) as boundary value methods

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(Advance online publication: 10 February 2018)

(BVMs) and obtained the generalized backward differentiation formulae (GBDF) with better stability properties than the BDF. This class of methods is

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h f_{n+v} \tag{7}$$

where

$$v = \begin{cases} \frac{k+2}{2} \ for\ even\ k \\ \frac{k+1}{2} \ for\ odd\ k \end{cases}$$

It is $0_{v,k-v}$-stable and $A_{v,k-v}$-stable for all $k \geq 1$ with $(v, k-v)$-boundary conditions and order $p = k$. A survey of some BVMs can be found in the literatures [12, 13, 14, 15, 16, 17, 33, 11, 1, 2, 3, 40, 32, 41]. In this paper second derivative generalized backward differentiation formulae (SDGBDF) shall be derived. This class of methods is an extention of GBDF proposed by [8] and [9]. The methods developed which are also applied as BVMs in the sense of [8] and [9] have improved order properties compared to the GBDF with respect to the steplength k and are suited for the solution of stiff IVPs in ODEs (1).

The paper is organized as follows. In section 2 we recall the main facts about BVMs. The stability of BVMs is discussed in section 3. Section 4 deals with the second derivative BVMs, the derivation and stability. Section 5 is devoted to the computational aspect for the implementation of the proposed class of methods to demonstrate how the class of methods are applied as BVMs. Numerical experiments are carried out in section 6. Finally, in section 7 the conclusion of the paper is given.

2 Boundary Value Methods (BVMs)

To obtain the numerical solution of (1) it is usual to use a k-step linear multistep formula (LMF),

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \tag{8}$$

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 $k_1 + k_2 = k$ then one may impose the k conditions for the LMF (8) by fixing the first $k_1(\leq k)$ values of the discrete solution $y_0, y_1, \ldots, y_{k_1-1}$ and the last $k_2 = k - k_1$ values $y_{N-k_2+1}, \ldots, y_N$ yielding the discrete problem

$$\sum_{i=-k_1}^{k_2} \alpha_{i+k_1} y_{n+i} = h \sum_{i=-k_1}^{k_2} \beta_{i+k_1} f_{n+i}, n = k_1, \ldots, N - k_2, \tag{9}$$

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

In this case the given continuous initial value problem (1) is approximated by means of a discrete boundary value problem. The resulting methods are BVMs with (k_1, k_2)-boundary conditions. Observe that for $k_1 = k$ and therefore $k_2 = 0$, one has the initial value methods (IVMs). So the class of IVMs is a subclass of BVMs for ODEs based on LMF [7]. The continuous problem (1) provides only the initial value y_0. In the sense of [7], to implement (9) as a BVM, the $k-1$ additional values $y_1, \ldots, y_{k_1-1},\ y_{N-k_2+1}, \ldots, y_N$ are obtained by introducing a set of $k-1$ additional equations which are derived by a set of $k_1 - 1$ additional initial methods

$$\sum_{i=0}^{k} \alpha_i^{(j)} y_i = h \sum_{i=0}^{k} \beta_i^{(j)} f_i\ , \quad j = 1, \ldots, k_1 - 1 \tag{10}$$

and k_2 final methods

$$\sum_{i=0}^{k} \alpha_{k-i}^{(j)} y_{N-i} = h \sum_{i=0}^{k} \beta_{k-i}^{(j)} f_{N-i}\ , \tag{11}$$

$$j = N - k_2 + 1, \ldots, N$$

The equations (9), (10) and (11) form a composite scheme assumed to be of the same order where (10) and (11) are the most suitable set of additional methods. The discrete problem generated by a k-step BVM with (k_1, k_2)-boundary conditions can be put in matrix form as

$$A_N \mathbf{y} - h B_N \mathbf{f} = \begin{pmatrix} \sum_{i=0}^{k_1-1} (\alpha_i y_i - h\beta_i f_i) \\ \vdots \\ \alpha_0 y_{k_1-1} - h\beta_0 f_{k_1-1} \\ 0 \\ \vdots \\ 0 \\ \alpha_k y_N - h\beta_k f_N \\ \vdots \\ \sum_{i=1}^{k_2} (\alpha_{k_1+i} y_{N-1+i} - h\beta_{k_1+i} f_{N-1+i}) \end{pmatrix} \tag{12}$$

where A_N and B_N are $(N+1) \times (N+1)$ matrices given in (39) and (40) respectively, $\mathbf{y} = (y_0, \ldots, y_N)^T$ is the discrete solution, $\mathbf{f} = (f_0, \ldots, f_N)^T$ and h is the step size. The matrix $A_N - qB_N$, where $q = h\lambda$, has a block quasi-Toeplitz structure which is as a result of the additional methods (10) and (11) in A_N and B_N as given in (12).

3 Stability of BVMs

In order to characterize the stability of the family of methods to be considered the definitions of zero-stability and absolute stability for LMM (8) are generalized to BVM by introducing the following two kinds of polynomials [6, 8]:

Definition 3. *Consider a polynomial $p(z)$ such that p is a function of a complex variable z, calculated by the formula:*

$$p(z) = \sum_{j=0}^{k} \alpha_j z^{k-j} = \alpha_0 z^k + \alpha_1 z^{k-1} + \ldots + \alpha_k \qquad (\alpha_0 \neq 0) \tag{13}$$

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

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

2. The polynomial $p(z)$ is called the Von Neumann polynomial if for all values of $i = 1,\ldots,k$ the condition $|z_i| \leq 1$ is satisfied ([37]).

Definition 4. *A polynomial $p(z)$ of degree $k = k_1 + k_2$ is a $S_{k_1k_2}$-polynomial if its roots are such that*

$|z_1| \leq |z_2| \leq \ldots \leq |z_{k_1}| < 1 < |z_{k_1+1}| \leq \ldots \leq |z_k|$

and it is a $N_{k_1k_2}$ - polynomial if

$|z_1| \leq |z_2| \leq \ldots \leq |z_{k_1}| \leq 1 < |z_{k_1+1}| \leq \ldots \leq |z_k|$ being simple the roots of unit modulus.

Observe that for $k_1 = k$ and $k_2 = 0$ a $N_{k_1k_2}$- polynomial reduces to a Von Neumann polynomial and a $S_{k_1k_2}$-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 (8). Thus $\prod(z,q) = \rho(z) - q\sigma(z), q = h\lambda$, is the stability polynomial when (8) is applied on $y' = \lambda y, Re(\lambda) < 0$. Then we have the following definitions (see [6, 7]):

Definition 5. *A BVM with (k_1, k_2)-boundary conditions is $O_{k_1k_2}$-stable if $\rho(z)$ is a $N_{k_1k_2}$ - polynomial.*

Observe that $O_{k_1k_2}$-stability reduces to the usual zero-stability from Definition 5. for LMM when $k_1 = k$ and $k_2 = 0$.

Definition 6. *(a) For a giving $q \in C$, a BVM with (k_1, k_2)-boundary conditions is (k_1, k_2)-absolutely stable if $\prod(z,q)$ is a $S_{k_1k_2}$-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 $D_{k_1k_2} = \{q \in C : \prod(z,q)$ is a $S_{k_1k_2}$-pololynomial$\}$. Here $\prod(z,q)$ is a polynomial of type $(k_1, 0, k_2)$

(c) A BVM with (k_1, k_2)-boundary conditions is said to be $A_{k_1k_2}$ -stable if $C^- \subseteq D_{k_1k_2}$.

4 Second Derivative BVMs, Derivation and Stability

The second derivative backward differentiation formulae (SDBDF) are based on the second derivative linear multistep formula (SDLMF) and can be defined generally as:

$$\sum_{i=0}^{k} \alpha_j y_{n+j} = h\beta_k f_{n+k} + h^2\gamma_k f'_{n+k} \qquad (14)$$

The conventional SDBDF provides 0-stable methods up to $k = 8$ and are 0-unstable for $k \geq 9$ with an order $p = k + 1$. Following the idea of Brugnano and Trigiante [6, 7, 8, 9], we rewrite (14) as:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_i f_{n+i} + h^2 f'_{n+i} \qquad (15)$$

where $i = 0(1)k$ and γ_k has been normalized to 1. The choice $i = k$ is widely used to derive the conventional SDBDF as IVMs. When (15) is used as BVMs with $i \neq k$, we gain the freedom of choosing the values of i which provide methods having the best stability properties for all values of $k \geq 1$. In fact this is the case if $i = v$ such that

$$v = \begin{cases} \frac{k+2}{2} & for\ even\ k \\ \frac{k+1}{2} & for\ odd\ k \end{cases} . \qquad (16)$$

Consequently (15) becomes

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_v f_{n+v} + h^2 f'_{n+v} \qquad (17)$$

where the $k + 2$ parameters allow the construction of methods of maximal order $p = k+1$. The class of methods (17) called second derivative generalized backward differentiation formulae (SDGBDF) must be used as BVMs with $(v, k - v)$ boundary conditions. These methods are found to be $0_{v,k-v}$-stable and $A_{v,k-v}$-stable for all $k \geq 1$ where v is the number of roots inside the unit circle and $k - v$ are the number of roots outside the unit circle. We rewrite the formula (17) as:

$$\sum_{j=0}^{k} \alpha_j y(x + jh) = h\beta_v y'(x + vh) + h^2 y''(x + vh). \qquad (18)$$

Expanding (18) in Taylor series and applying the method of undetermined coefficients yields a system of linear equations for the coefficients α_j and β_v (see [38] and [18]). These coefficients are in Tables 7 and 8 for $k = 1(1)10$. According to [37] and [27] the local truncation error associated with (17) is the linear difference operator

$$\begin{aligned} &L[y(x); h] = \textstyle\sum_{j=0}^{k} \alpha_j y(x + jh) \\ &-h\beta_v y'(x + vh) - h^2 y''(x + vh). \end{aligned} \qquad (19)$$

Assuming that $y(x)$ is sufficiently differentiable, we can find the Taylor series expansion of the terms in (19) about the point x to obtain the expression

$$\begin{aligned} &L[y(x); h] = \\ &C_0 y(x) + C_1 h y'(x) + \cdots + C_q h^q y^{(q)}(x) + \cdots \end{aligned} \qquad (20)$$

where

$$C_0 = \sum_{j=0}^{k} \alpha_j, \quad C_1 = \sum_{j=1}^{k} j\alpha_j + \beta_v, \quad , \quad \cdots$$

$$C_q = \sum_{j=1}^{k} \frac{j^q \alpha_j}{q!} + \frac{\beta_v v^{q-1}}{(q-1)!} - \frac{v^{q-2}}{(q-2)!}$$

We say that (17) has order p if

$$C_j = 0,\ j = 0(1)p \ \ and \ \ C_{p+1} \neq 0, \tag{21}$$

see [31]. The C_{p+1} is the error constant and $C_{p+1}h^{p+1}y^{p+1}(x)$ is the principle local truncation error at the point x. The order equations (21) is equivalent to

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & \dots & 1 & 0 \\ 0 & 1 & 2 & 3 & 4 & \dots & k & 1 \\ 0 & 1 & 2^2 & 3^2 & 4^2 & \dots & k^2 & 2v \\ 0 & 1 & 2^3 & 3^3 & 4^3 & \dots & k^3 & 3v^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 1 & 2^q & 3^q & 4^q & \dots & k^q & qv^{q-1} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_k \\ \beta_v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \\ 6v \\ \vdots \\ q(q-1)v^{q-2} \end{bmatrix} \tag{22}$$

The order and the error constant of the SDGBDF (17) are shown in tables 7 and 8 for $k = 1(1)10$.

For the numerical solution of (1) the second derivative BVMs with (k_1, k_2)-boundary conditions, the main method

$$\sum_{i=-k_1}^{k_2} \alpha_{i+k_1} y_{n+i} = h \sum_{i=-k_1}^{k_2} \beta_{i+k_1} f_{n+i} + h^2 \sum_{i=-k_1}^{k_2} \lambda_{i+k_1} f'_{n+i}\ , \tag{23}$$

$$n = k_1, \dots, N - k_2$$

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

together with $k_1 - 1$ additional initial methods

$$\sum_{i=0}^{k} \alpha_i^{(j)} y_i = h \sum_{i=0}^{k} \beta_i^{(j)} f_i + h^2 \sum_{i=0}^{k} \lambda_i^{(j)} f'_i\ , \tag{24}$$

$$j = 1, \dots, k_1 - 1$$

and k_2 final methods

$$\left\{ \begin{array}{l} \sum_{i=0}^{k} \alpha_{k-i}^{(j)} y_{N-i} = h \sum_{i=0}^{k} \beta_{k-i}^{(j)} f_{N-i} \\ +h^2 \sum_{i=0}^{k} \lambda_{k-i}^{(j)} f'_{N-i}\ , \quad j = N, \dots, N + k_2 - 1 \end{array} \right. \tag{25}$$

can be expressed as

$$A_N\mathbf{y} - hB_N\mathbf{f} - h^2 C_N \mathbf{f'} = \begin{pmatrix} \sum_{i=0}^{k_1-1} (\alpha_i y_{n+i} - h\beta_i f_{n+i} - h^2 \lambda_i f'_{n+i}) \\ \vdots \\ \alpha_0 y_{n+k_1-1} - h\beta_0 f_{n+k_1-1} - h^2 \lambda_0 f'_{n+k_1-1} \\ 0 \\ \vdots \\ 0 \\ \alpha_k y_{n+N} - h\beta_k f_{n+N} - h^2 \lambda_k f'_{n+N} \\ \vdots \\ \sum_{i=1}^{k_2} (\alpha_{k_1+i} y_{n+N-1+i} - h\beta_{k_1+i} \times \\ f_{n+N-1+i} - h^2 \lambda_{k_1+i} f'_{n+N-1+i}) \end{pmatrix} \tag{26}$$

where A_N and B_N are defined similarly as in (12), while C_N is given in (41), $\mathbf{y} = (y_0, \dots, y_N)^T$ is the discrete solution, $\mathbf{f}$ and $\mathbf{f'}$ are the first and second derivatives respectively, h is the step size and A_N, B_N and C_N are $(N+1) \times (N+1)$ matrices with the same structure as those in (12).

To analyze the stability of a specific method (26), (see, [30]) we apply (23) on the test problem

$$y' = \lambda y, \quad y'' = \lambda^2 y \tag{27}$$

to determine its boundary locus. The class of methods (17) yields the characteristics equation:

$$\sum_{j=0}^{k} \alpha_j z^j - (q\beta_v + q^2) z^v = 0, \quad q = \lambda h, \quad q \in C \tag{28}$$

where v is defined as in (16). Letting $z = e^{i\theta}$ we obtain two roots (since (28) is quadratic in q) for corresponding values of k and v to give the stability regions defined by q given in Figures 1 and 2 for odd and even values of k respectively. Compared with the generalization of the BDF by Brugnano and Trigiante [8] discussed in section 1 the proposed class of methods (17) are found to have higher order $p = k + 1$ and a smaller error constant for corresponding values of the steplength k, although with need to compute the second derivative for which it is not expensive for some autonomous stiff systems.

5 Implementation Procedure

In this section the implementation procedure for the SDGBDF(17) of order 4 and 5 as BVMs in the sense of Brugnano and Trigiante [7, 8] is presented. The proposed class of methods (17) is used with the following additional initial methods:

$$\sum_{j=0}^{k} \alpha_j^* y_j = h\beta_i f_i + h^2 f'_i, \quad i = 1, 2, \cdots, v - 1 \tag{29}$$

and final methods:

$$\sum_{j=0}^{k} \alpha_j^* y_j = h\beta_i f_i + h^2 f'_i, \quad i = v + 1, \cdots, N \tag{30}$$

The SDGBDF (17) of order 4 which is $A_{2,1}$-stable and $0_{2,1}$-stable with $(2, 1)$-boundary conditions requires two initial methods (y_0 is already provided by the initial value defining the ODE (1)) and one final method. The fourth order SDGBDF (17) is given as:

$$-\frac{1}{6} y_n + 2y_{n+1} - \frac{5}{2} y_{n+2} + \frac{2}{3} y_{n+3} = -hf_{n+2} + h^2 f'_{n+2} \tag{31}$$

The main method (31) can be written in the form

$$-\frac{1}{6} y_{n-2} + 2y_{n-1} - \frac{5}{2} y_n + \frac{2}{3} y_{n+1} = -hf_n + h^2 f'_n \tag{32}$$

$n = 2, \cdots, N - 1$

and used with the following initial method

$$\frac{2}{3}y_0 - \frac{5}{2}y_1 + 2y_2 - \frac{1}{6}y_3 = hf_1 + h^2 f_1' \qquad (33)$$

and final method

$$\frac{2}{9}y_{N-3} - \frac{3}{2}y_{N-2} + 6y_{N-1} - \frac{85}{18}y_N = -\frac{11}{3}hf_N + h^2 f_N' \qquad (34)$$

Similarly the SDGBDF (17) of order 5

$$\left\{ \begin{array}{l} \frac{1}{18}y_n - \frac{1}{2}y_{n+1} + 3y_{n+2} - \frac{55}{18}y_{n+3} + \frac{1}{2}y_{n+4} \\ = -\frac{5}{3}hf_{n+3} + h^2 f_{n+3}' \end{array} \right. \qquad (35)$$

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

with the initial methods

$$\frac{1}{2}y_0 - \frac{55}{18}y_1 + 3y_2 - \frac{1}{2}y_3 + \frac{1}{18}y_4 = \frac{5}{3}hf_1 + h^2 f_1' \qquad (36)$$

and

$$-\frac{1}{12}y_0 + \frac{4}{3}y_1 - \frac{5}{2}y_2 + \frac{4}{3}y_3 - \frac{1}{12}y_4 = 2h^2 f_2' \qquad (37)$$

and the final method

$$\left\{ \begin{array}{l} -\frac{1}{8}y_{N-4} + \frac{8}{9}y_{N-3} - 3y_{N-2} + 8y_{N-1} - \frac{415}{72}y_N \\ = -\frac{25}{6}hf_N + h^2 f_N' \end{array} \right. \qquad (38)$$

will be taken together as a BVM.

The methods (31 and 35) are implemented as BVMs efficiently by composing the main methods and the additional methods as simultaneous numerical integrators for the IVP(1). In particular for linear problems, we can solve (1) directly from the start with Gaussian elimination partially using pivoting and for nonlinear problems we can use a modified Newton-Raphson method. In each case, the main methods 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 $\{y_n\}, \{y_n'\}, n = 0, \ldots, N$, where the single block matrix equation is solved while adjusting for boundary conditions ([35]).

6 Numerical Experiments with SDGBDF

We consider the following stiff problems (linear and nonlinear) to illustrate the implementation and examine the accuracy of the SDGBDF (17) of orders p=4 (31) and 5 (35) implemented as block methods. The fourth order method (17) and the fifth order method (17) are denoted by SDGBDF4 and SDGBDF5 respectively.

Problem 1: A linear stiff problem, see [4, 10, 25, 43]

$$y_1' = -21y_1 + 19y_2 - 20y_3, \qquad y_1(0) = 1,$$

$$y_2' = 19y_1 - 21y_2 + 20y_3, \qquad y_2(0) = 0,$$

$$y_3' = 40y_1 - 40y_2 + 40y_3, \qquad y_3(0) = -1.$$

The SDGBDF4 is applied to this problem and the maximum absolute errors ($|y(x) - y_n|$) in the interval $0 < x < 10$ are compared with the Adams type block method of Akinfenwa [4] (ATBM7), the generalized backward differentiation formula of Brugnano and Trigiante [10](GBDF8) and the $L(\alpha)$-stable block multistep method of Ehigie and Okunuga [25] denoted by EH-OK5. The rate of convergence, $Rate_h = log_2(\frac{err_2h}{err_h})$ where err_h is the maximum absolute error at steplength $h = \frac{1}{2^n.100}, n = 0, 1, 2, 3$ and 4 , is used to verify the order of the methods. Also in comparison with the $CBDF_5$ of degree $s = 5$ in Ramos and Garcia-Rubio [43], the AbsErr(t_f) is obtained by the SDGBDF4 in the interval $0 \leq x \leq 1$. It is observed that the new method even though it is of order 4 performs better than the EH-OK5, the ATBM7 and the GBDF8 of orders 5, 7 and 8 respectively. The details of the numerical results are displayed in Table 1. In Table 2, it is noticed that the SDGBDF4 is comparable with the EH-OK5 in [25] and the $CBDF_5$ in [43].

Table 1: Maximum absolute error, $Max_{1<i<N}|y_i(x) - y_{i,n}|$ for problem 1, $h = \frac{1}{2^n.100}$

n	SDGBDF4 (Rate)	EH-OK5 (Rate)	GBDF8 (Rate)	ATBM7 (Rate)
0	2.28×10^{-17}	3.21×10^{-13}	1.19×10^{-3}	3.95×10^{-6}
1	1.56×10^{-18} (3.87)	1.01×10^{-14} (4.99)	1.39×10^{-5} (6.42)	2.91×10^{-8} (7.08)
2	1.02×10^{-19} (3.93)	3.18×10^{-16} (4.99)	1.08×10^{-7} (7.00)	2.21×10^{-10} (7.06)
3	6.21×10^{-21} (4.04)	9.96×10^{-18} (5.00)	1.08×10^{-9} (6.64)	6.65×10^{-13} (8.36)
4	9.45×10^{-23} (6.04)	3.11×10^{-19} (5.00)	9.41×10^{-12} (6.84)	2.69×10^{-15} (7.95)

Table 2: Numerical results in comparison with $CBDF_5$ and EH-OK5 for problem 1 the interval $0 \leq x \leq 1$

Steps	SDGBDF4 (Rate)	EH-OK5 (Rate)	$CBDF_5$ (Rate)
20	1.12×10^{-11}	3.04×10^{-11}	4.12×10^{-12}
40	7.01×10^{-13} (4.00)	9.75×10^{-13} (4.96)	1.33×10^{-12} (4.95)
80	4.47×10^{-14} (3.97)	2.25×10^{-14} (5.43)	4.31×10^{-15} (4.95)
160	1.47×10^{-15} (4.93)	9.69×10^{-16} (4.53)	2.55×10^{-15} (0.75)

Problem 2: Non-linear stiff system solved by Wu and Xia [44]

$$y_1' = -1002y_1 + 1000y_2^2, \qquad y_1(0) = 1,$$

$$y_2' = y_1 - y_2(1 + y_2), \qquad y_2(0) = 1,$$

The exact solution of the system is given by

$$y_1(x) = e^{-2x}, \quad y_2(x) = e^{-x}$$

Problem 2 is solved using SDGBDF5 with a steplength $h = 0.008$ in the range $0 \le x \le 1$. The maximum error $(\text{Max}|y_i - y(x_i)|)$ of the method is given in Table 3. From Table 3, it is obvious that the new method of order 5 is better than the methods of Ehigie et al [24] and Wu-Xia [44] and very comparable with the method of Jator and Sahi [36] which are of orders 5, 6 and 8 respectively.

Problem 3: Singularly Perturbed Problem

Table 3: Maximum error, $\text{Max}|y_i - y(x_i)|$, for problem 2

Method	N	h	y_1 $(\text{Max}\|y_i - y(x_i)\|)$	y_2 $(\text{Max}\|y_i - y(x_i)\|)$
SDGBDF5	125	0.008	1.80×10^{-15}	6.11×10^{-16}
Ehigie et al (BVM3)	125	0.008	3.88×10^{-14}	3.10×10^{-14}
Jator-Sahi	125	0.008	1.63×10^{-14}	0.00
Wu-Xia	500	0.002	2.56×10^{-07}	8.02×10^{-08}

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

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

The exact solution is $y_1 = e^{-2t}$, $y_2 = e^{-t}$, see [30]. The SDGBDF4 and the SDGBDF5 are applied to Problem 3 and the results are compared with the theoretical solution. The SDGBDF5 performs better than the SDGBDF4 as expected, see Table 4. Furthermore, take note that the graphs of the exact and the numerical solutions in Figures 3 and 4 coincide.

Table 4: Absolute error in problem 3, $h = 0.01$, Error y_i=$|y_i - y(x_i)|$, $i = 1, 2$

x	y_i	Error in SDGBDF4	Error in SDGBDF5
1.0	y_1	3.06126×10^{-11}	3.43744×10^{-11}
	y_2	4.22623×10^{-11}	4.96455×10^{-11}
2.0	y_1	1.03235×10^{-11}	5.15573×10^{-12}
	y_2	3.96899×10^{-11}	1.91052×10^{-11}
3.0	y_1	2.39019×10^{-12}	6.49362×10^{-13}
	y_2	2.40044×10^{-11}	6.79007×10^{-12}
4.0	y_1	4.31932×10^{-13}	9.57145×10^{-14}
	y_2	1.20298×10^{-11}	2.61306×10^{-12}
5.0	y_1	8.00396×10^{-14}	1.20228×10^{-14}
	y_2	5.82196×10^{-12}	9.28587×10^{-13}
6.0	y_1	1.27167×10^{-14}	1.77133×10^{-15}
	y_2	2.56518×10^{-12}	3.57306×10^{-13}
7.0	y_1	2.18299×10^{-15}	2.22482×10^{-16}
	y_2	1.15005×10^{-12}	1.26970×10^{-13}
8.0	y_1	3.27871×10^{-16}	3.27798×10^{-17}
	y_2	4.79014×10^{-13}	4.88578×10^{-14}
9.0	y_1	4.83562×10^{-17}	4.11682×10^{-18}
	y_2	1.95919×10^{-13}	1.73602×10^{-14}
10.0	y_1	7.87909×10^{-18}	6.06524×10^{-19}
	y_2	8.33725×10^{-14}	6.67981×10^{-15}

Problem 4: Van der Pol equations, see [30] (nonlinear problem)

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

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

For problem 4, it is clearly seen from Table 5 and Figures 5 and 6 that the proposed class of methods compares favorably with the solution from the Ode15s in MATLAB.

Problem 5: Robertson's equation, see [30] (nonlinear problem)

$$y_1' = -0.04y_1 + 10^4 y_2 y_3, \quad y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3\times10^7 y_2^2,$$

$$y_3' = 3\times10^7 y_2^2, \quad y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0.$$

Problem 5 is solved by the SDGBDF4 and the SDGBDF5 and the results are compared with the solution from the Ode15s in MATLAB. It is observed from Table 6 and Figures 7 and 8 that the new methods are very comparable with the Ode15s in MATLAB.

Table 5: Errors in problem 4 using the modulus of the solution of SDGBDF minus the solution of Ode15s, $h = 0.001$. Error $y_i = |y_{iSDGBDF} - y_{iOde15s}|$, $i = 1, 2$

x	y_i	Error in SDGBDF4	Error in SDGBDF5
1.0	y_1	1.32308×10^{-4}	1.82747×10^{-5}
	y_2	8.31878×10^{-6}	1.09583×10^{-6}
5.0	y_1	3.36208×10^{-4}	1.47667×10^{-4}
	y_2	2.22430×10^{-5}	3.98291×10^{-6}
10.0	y_1	3.67025×10^{-5}	2.25767×10^{-4}
	y_2	1.98333×10^{-6}	1.32565×10^{-5}
15.0	y_1	2.46188×10^{-5}	6.92917×10^{-4}
	y_2	3.09782×10^{-5}	7.75023×10^{-5}
20.0	y_1	9.04906×10^{-5}	2.00872×10^{-4}
	y_2	1.10280×10^{-5}	6.98618×10^{-6}

Table 6: Errors in problem 5 using the modulus of the solution of SDGBDF minus the solution of Ode15s, $h = 0.0001$. Error $y_i = |y_{iSDGBDF} - y_{iOde15s}|$, $i = 1, 2, 3$

x	y_i	Error in SDGBDF4	Error in SDGBDF5
1.0	y_1	2.31233×10^{-5}	6.11248×10^{-6}
	y_2	3.68698×10^{-9}	9.74789×10^{-10}
	y_3	2.31270×10^{-5}	6.11346×10^{-6}
3.0	y_1	3.91192×10^{-6}	3.91187×10^{-6}
	y_2	4.93245×10^{-10}	4.93239×10^{-10}
	y_3	3.91241×10^{-6}	3.91236×10^{-6}
5.0	y_1	1.02179×10^{-6}	1.02175×10^{-6}
	y_2	2.95023×10^{-10}	2.95027×10^{-10}
	y_3	1.02149×10^{-6}	1.02146×10^{-6}
7.0	y_1	4.48772×10^{-5}	4.48771×10^{-5}
	y_2	4.22263×10^{-9}	4.22262×10^{-9}
	y_3	4.48814×10^{-5}	4.48814×10^{-5}
10.0	y_1	7.35061×10^{-5}	7.35060×10^{-5}
	y_2	5.76555×10^{-9}	5.76555×10^{-9}
	y_3	7.35118×10^{-5}	7.35118×10^{-5}

Table 7: The Coefficients, Error Constant (EC) and Order p of SDGBDF(18) for $k = 1(1)10$

k	v	α_0	α_1	α_2	α_3	α_4	α_5	α_6
1	1	2	-2	0	0	0	0	0
2	2	$-\frac{1}{2}$	4	$-\frac{7}{2}$	0	0	0	0
3	2	$-\frac{1}{6}$	2	$-\frac{5}{2}$	$\frac{2}{3}$	0	0	0
4	3	$\frac{1}{18}$	$-\frac{1}{2}$	3	$-\frac{55}{18}$	$\frac{1}{2}$	0	0
5	3	$\frac{1}{45}$	$-\frac{1}{4}$	2	$-\frac{49}{18}$	1	$-\frac{1}{20}$	0
6	4	$-\frac{1}{120}$	$\frac{4}{45}$	$-\frac{1}{2}$	$\frac{8}{3}$	$-\frac{217}{72}$	$\frac{4}{5}$	$-\frac{1}{30}$
7	4	$-\frac{1}{280}$	$\frac{2}{45}$	$-\frac{3}{10}$	2	$-\frac{205}{72}$	$\frac{6}{5}$	$-\frac{1}{10}$
8	5	$\frac{1}{700}$	$-\frac{1}{56}$	$\frac{1}{9}$	$-\frac{1}{2}$	$\frac{5}{2}$	$-\frac{5449}{1800}$	1
9	5	$\frac{1}{1575}$	$-\frac{1}{112}$	$\frac{4}{63}$	$-\frac{1}{3}$	2	$-\frac{5269}{1800}$	$\frac{4}{3}$
10	6	$-\frac{1}{3780}$	$\frac{2}{525}$	$-\frac{3}{112}$	$\frac{8}{63}$	$-\frac{1}{2}$	$\frac{12}{5}$	$-\frac{5489}{1800}$

Table 8: Table 7 continued

k	v	α_7	α_8	α_9	α_{10}	β_v	γ_v	EC	p
1	1	0	0	0	0	-2	1	$\frac{1}{3}$	2
2	2	0	0	0	0	-3	1	$\frac{1}{6}$	3
3	2	0	0	0	0	-1	1	$-\frac{1}{30}$	4
4	3	0	0	0	0	$-\frac{5}{3}$	1	$-\frac{1}{60}$	5
5	3	0	0	0	0	$-\frac{2}{3}$	1	$\frac{1}{210}$	6
6	4	0	0	0	0	$-\frac{7}{6}$	1	$\frac{1}{420}$	7
7	4	$\frac{2}{315}$	0	0	0	$-\frac{1}{2}$	1	$-\frac{1}{1260}$	8
8	5	$-\frac{1}{14}$	$\frac{1}{252}$	0	0	$-\frac{9}{10}$	1	$-\frac{1}{2520}$	9
9	5	$-\frac{1}{7}$	$\frac{1}{63}$	$-\frac{1}{1008}$	0	$-\frac{2}{5}$	1	$\frac{1}{6930}$	10
10	6	$\frac{8}{7}$	$-\frac{3}{28}$	$\frac{2}{189}$	$-\frac{1}{1680}$	$-\frac{11}{15}$	1	$\frac{1}{13860}$	11

$$A_N = \begin{pmatrix}
1 & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & \cdots & 0 \\
\alpha_0^{(1)} & \alpha_1^{(1)} & \alpha_2^{(1)} & \alpha_3^{(1)} & \cdots & \alpha_k^{(1)} & 0 & \cdots & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \cdots & \vdots \\
\alpha_0^{(k_1-1)} & \alpha_1^{(k_1-1)} & \alpha_2^{(k_1-1)} & \alpha_3^{(k_1-1)} & \cdots & \alpha_k^{(k_1-1)} & \vdots & \cdots & \cdots & \vdots \\
\alpha_0 & \alpha_1 & \alpha_2 & \alpha_3 & \cdots & \alpha_k & 0 & \cdots & \cdots & 0 \\
0 & \alpha_0 & \alpha_1 & \alpha_2 & \cdots & \alpha_{k-1} & \alpha_k & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & 0 & \alpha_0 & \cdots & \cdots & \cdots & \cdots & \alpha_k \\
\vdots & \ddots & \ddots & \vdots & \alpha_0^{(N-k_2+1)} & \cdots & \cdots & \cdots & \cdots & \alpha_k^{(N-k_2+1)} \\
\vdots & \ddots & \ddots & \vdots & \vdots & \cdots & \cdots & \cdots & \cdots & \vdots \\
0 & \cdots & \cdots & 0 & \alpha_0^{(N)} & \cdots & \cdots & \cdots & \cdots & \alpha_k^{(N)}
\end{pmatrix} \quad (39)$$

$$B_N = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & \cdots & 0 \\ \beta_0^{(1)} & \beta_1^{(1)} & \beta_2^{(1)} & \beta_3^{(1)} & \cdots & \beta_k^{(1)} & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \cdots & \vdots \\ \beta_0^{(k_1-1)} & \beta_1^{(k_1-1)} & \beta_2^{(k_1-1)} & \beta_3^{(k_1-1)} & \cdots & \beta_k^{(k_1-1)} & \vdots & \cdots & \cdots & \vdots \\ \beta_0 & \beta_1 & \beta_2 & \beta_3 & \cdots & \beta_k & 0 & \cdots & \cdots & 0 \\ 0 & \beta_0 & \beta_1 & \beta_2 & \cdots & \beta_{k-1} & \beta_k & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & \beta_0 & \cdots & \cdots & \cdots & \cdots & \beta_k \\ \vdots & \ddots & \ddots & \vdots & \beta_0^{(N-k_2+1)} & \cdots & \cdots & \cdots & \cdots & \beta_k^{(N-k_2+1)} \\ \vdots & \ddots & \ddots & \vdots & \vdots & \cdots & \cdots & \cdots & \cdots & \vdots \\ 0 & \cdots & \cdots & 0 & \beta_0^{(N)} & \cdots & \cdots & \cdots & \cdots & \beta_k^{(N)} \end{pmatrix} \tag{40}$$

$$C_N = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & \cdots & 0 \\ \lambda_0^{(1)} & \lambda_1^{(1)} & \lambda_2^{(1)} & \lambda_3^{(1)} & \cdots & \lambda_k^{(1)} & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \cdots & \vdots \\ \lambda_0^{(k_1-1)} & \lambda_1^{(k_1-1)} & \lambda_2^{(k_1-1)} & \lambda_3^{(k_1-1)} & \cdots & \lambda_k^{(k_1-1)} & \vdots & \cdots & \cdots & \vdots \\ \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 & \cdots & \lambda_k & 0 & \cdots & \cdots & 0 \\ 0 & \lambda_0 & \lambda_1 & \lambda_2 & \cdots & \lambda_{k-1} & \lambda_k & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & \lambda_0 & \cdots & \cdots & \cdots & \cdots & \beta_k \\ \vdots & \ddots & \ddots & \vdots & \lambda_0^{(N)} & \cdots & \cdots & \cdots & \cdots & \lambda_k^{(N)} \\ \vdots & \ddots & \ddots & \vdots & \vdots & \cdots & \cdots & \cdots & \cdots & \vdots \\ 0 & \cdots & \cdots & 0 & \lambda_0^{(N+k_2-1)} & \cdots & \cdots & \cdots & \cdots & \lambda_k^{(N+k_2-1)} \end{pmatrix} \tag{41}$$

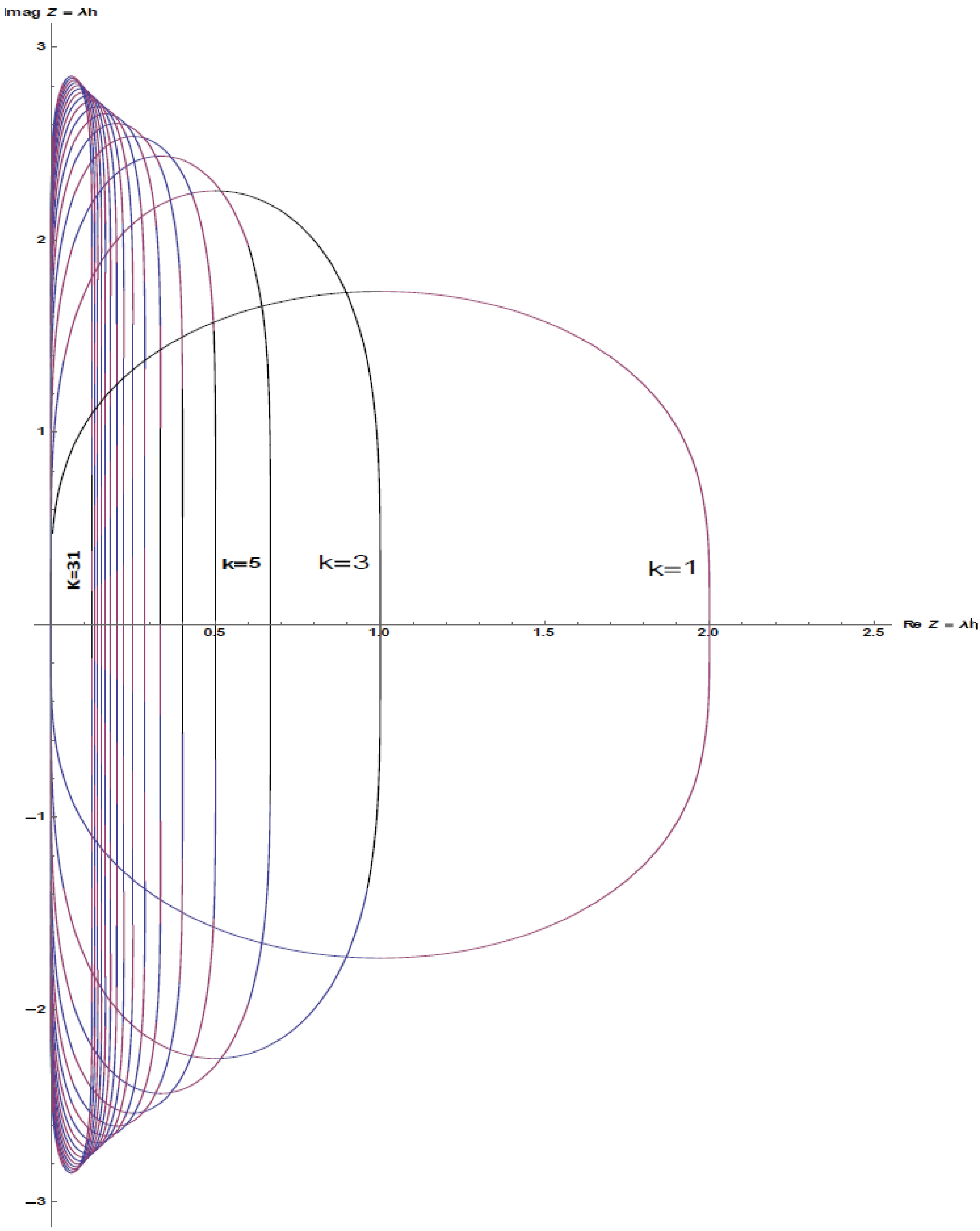

Figure 1: Stability region (exterior of closed curves) of (17), k=1 (2) 31

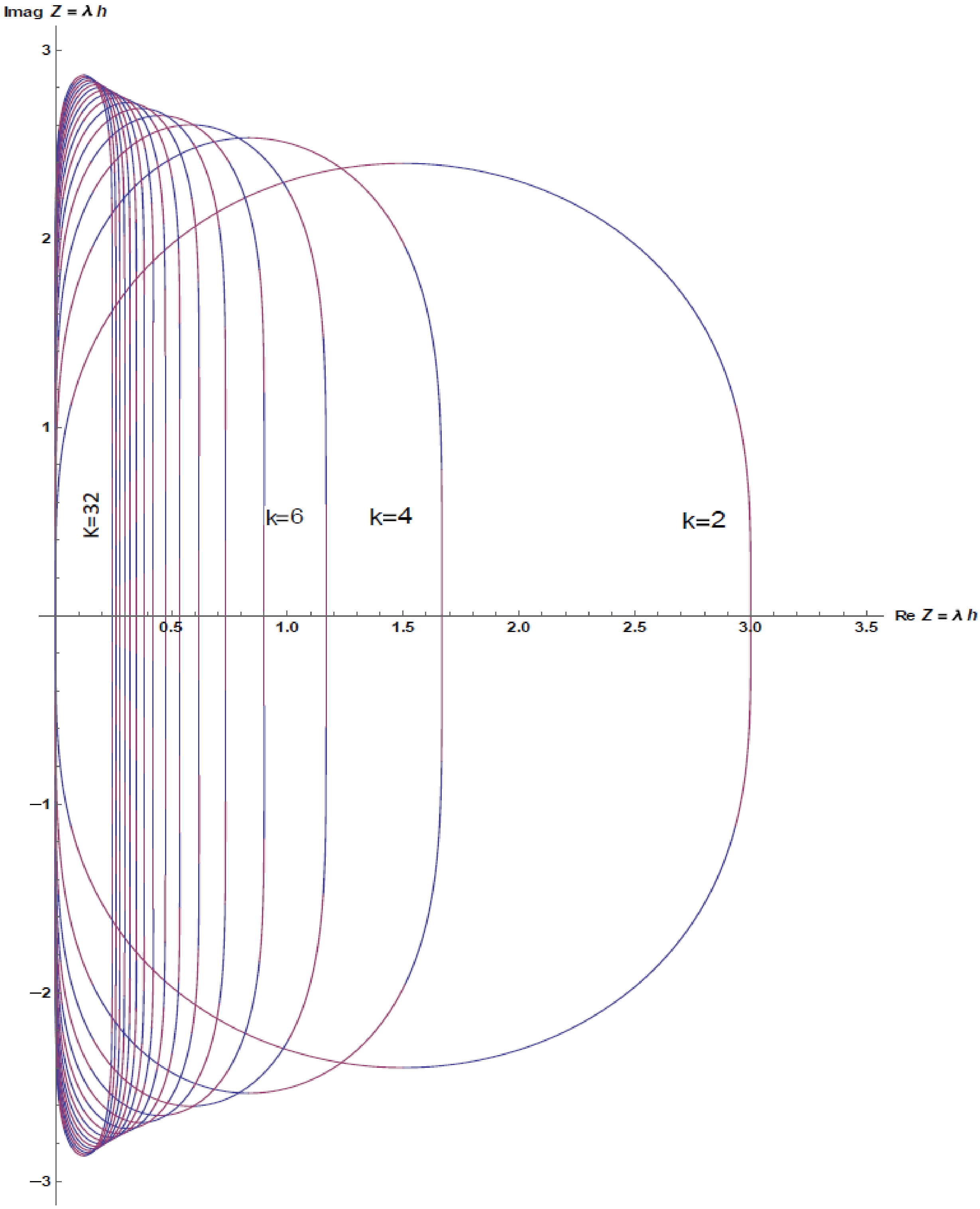

Figure 2: Stability region (exterior of closed curves) of (17), k=2 (2) 32

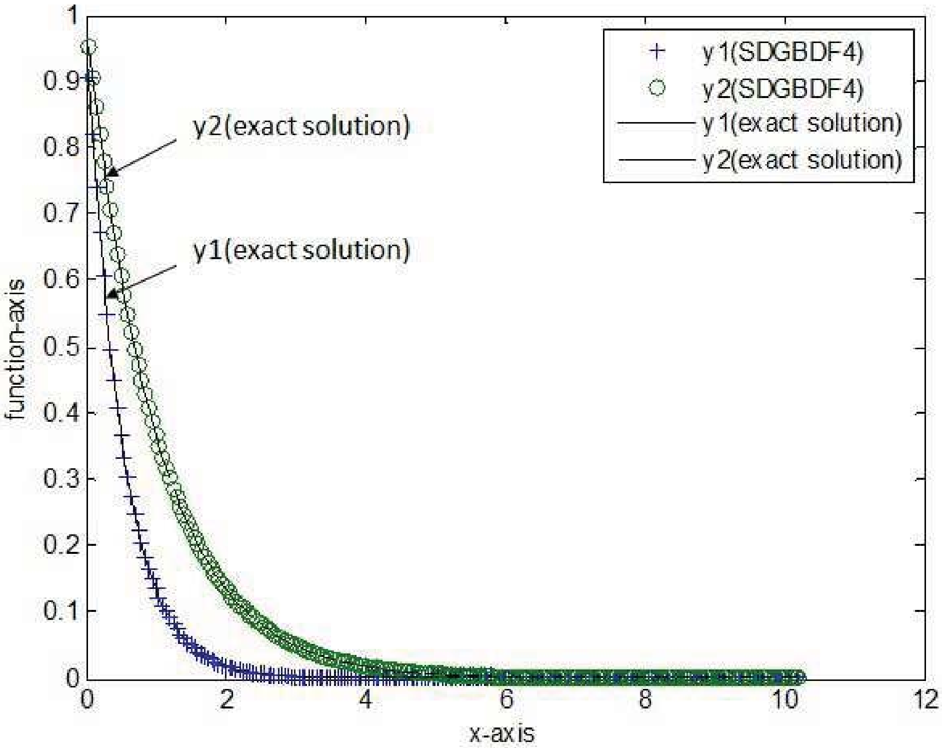

Figure 3: Numerical Results for Problem 3 with SDGBDF4, h=0.01

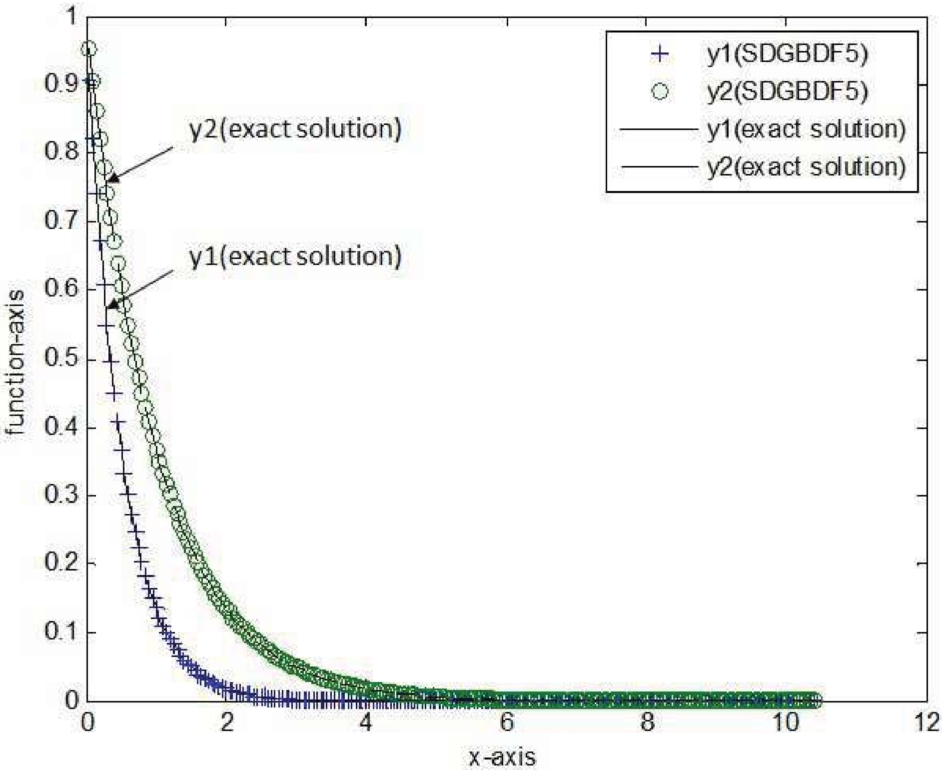

Figure 4: Numerical Results for Problem 3 with SDGBDF5, h=0.01

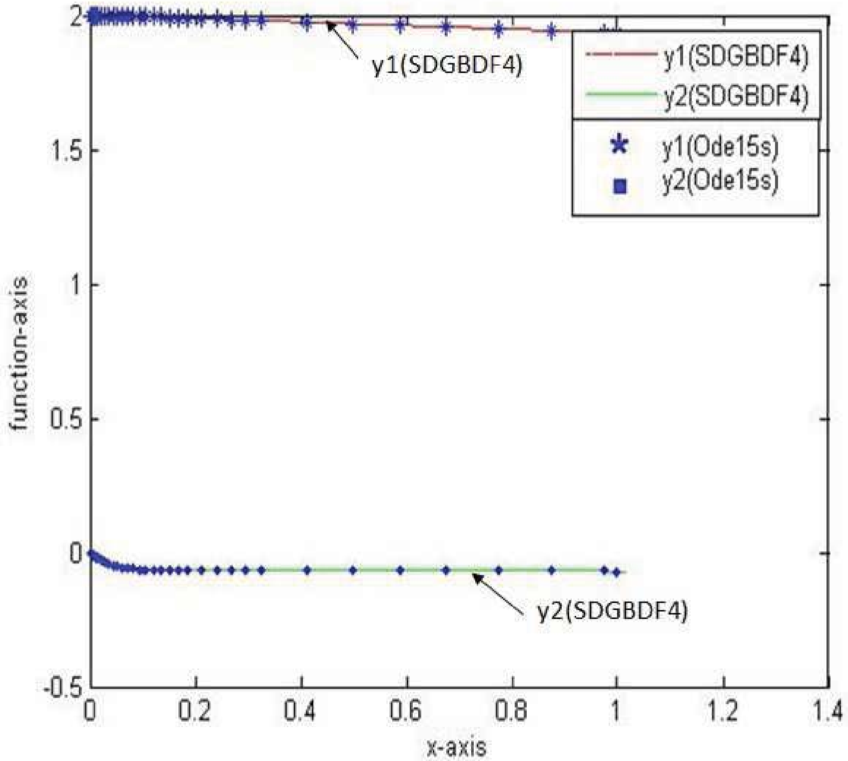

Figure 5: Numerical Results for Problem 4 with SDGBDF4, h=0.001

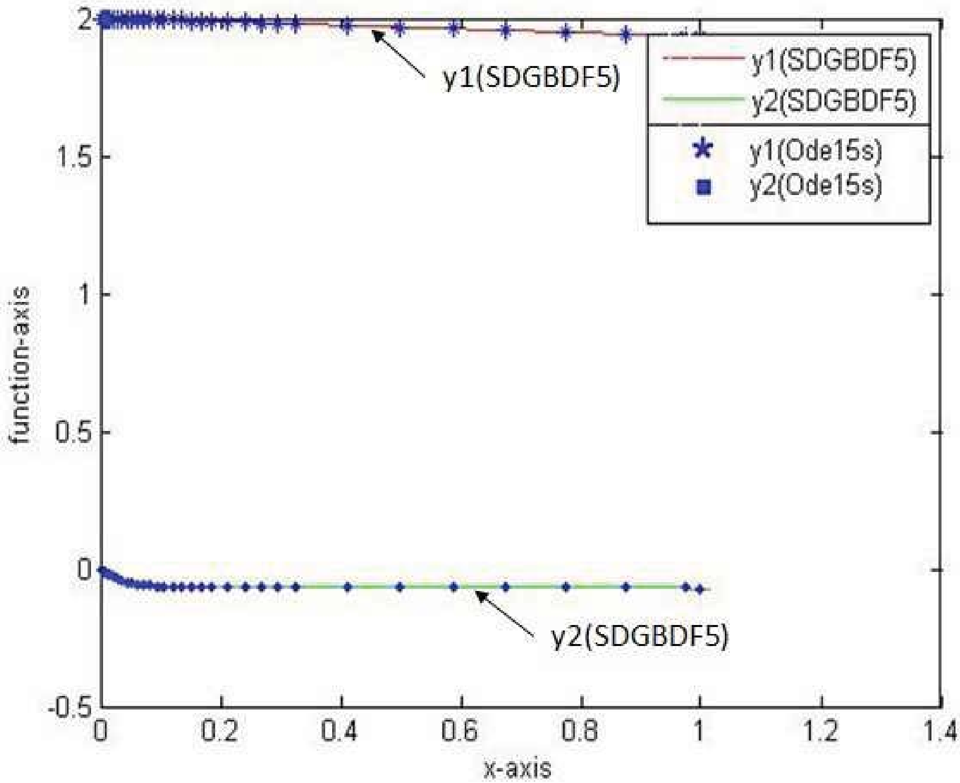

Figure 6: Numerical Results for Problem 4 with SDGBDF5, h=0.001

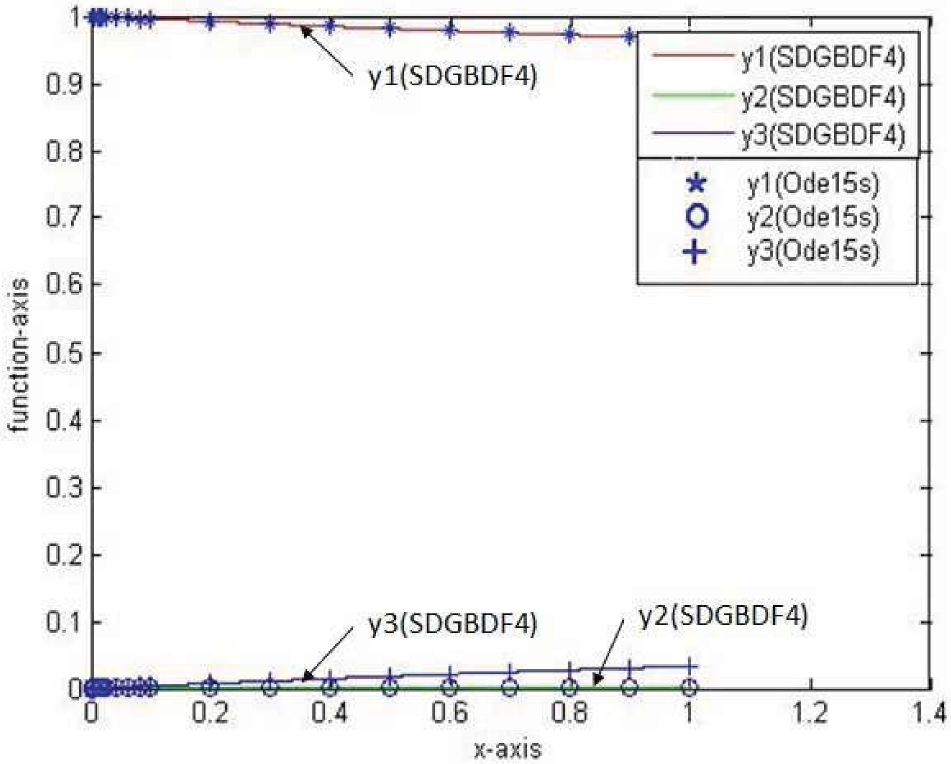

Figure 7: Numerical Results for Problem 5 with SDGBDF4, h=0.0001

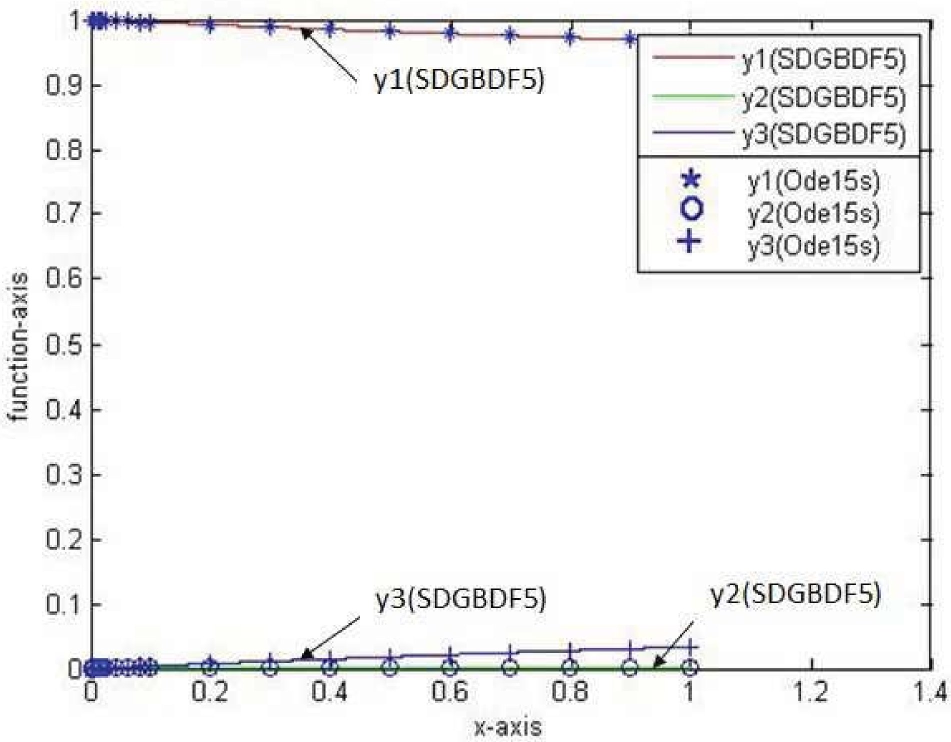

Figure 8: Numerical Results for Problem 5 with SDGBDF5, h=0.0001

7 Conclusion

The second derivative generalized backward differentiation formulae (SDGBDF) have been introduced in section (4). This class of methods is $A_{v,k-v}$-stable and $0_{v,k-v}$-stable with (v, k-v)-boundary conditions for values of $k \geq 1$ with order $p = k + 1$. The new class of methods is found to be suitable for the solution of stiff IVPs in ODEs for reason of their stability. The class of methods (17) also finds application in the solution of boundary value problems, see [35, 39].

Acknowledgement

The authors are grateful to Prof. M.N.O. Ikhile (Director of ARLAB) and the anonymous reviewers for comments that have improved the quality of this work.

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