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SECOND DERIVATIVE GENERALIZED EXTENDED BACKWARD DIFFERENTIATION FORMULAS FOR STIFF PROBLEMS

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ABSTRACT. This paper presents second derivative generalized extended backward differentiation formulas (SDGEBDFs) based on the second derivative linear multi-step formulas of Cash [1]. This class of second derivative linear multistep formulas is implemented as boundary value methods on stiff problems. The order, error constant and the linear stability properties of the new methods are discussed.

1. INTRODUCTION

Many practical models in different application areas such as chemical engineering, biology, circuit theory and other related disciplines often leads to a system of ordinary differential equations (ODEs), which are stiff [2]. The Runge-Kutta methods (RKMs) and linear multistep methods (LMMs) in [2, 3, 4, 5] are popular methods for generating the numerical solutions of stiff initial value problems (IVPs) in ODEs

$$y'(t) = f(t, y(t)), \quad t \in (t_0, T), \quad y(t_0) = y_0, \quad y(t) \in R^v, \\ f(t, y(t)) \in R^v, \quad t \in R, \quad v = 1, 2, ... \tag{1.1}$$

Although, the implicit Runge-Kutta methods have higher order A-stable methods for a given number of stages compared to LMMs,with same step number, but the computational cost on implementation is very high. The linear multistep methods

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}, \quad k \geq 1, \tag{1.2}$$

are relatively less expensive to implement, but suffer Dahlquist order and stability barrier [6] which state that the order of a $k-$step LMM can not exceed $p = k + 1$ (for k odd) or $p = k + 2$ (for k even) for zero-stability and the order of A-stable LMMs cannot exceed $p = 2$ (trapezoidal

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rule with error constant $C_{p+1} = \frac{1}{12}$). In this regards, these barriers have been overcome by introducing second derivative linear multistep methods (SDLMMs) which is a special class of Obreckoff [7] to obtain methods that are highly stable and at the same time with order exceeding $p = 2$ (See, [3, 8, 9, 10]). In particular, Cash [1] improved the second derivative backward differentiation formulas (SDBDF)

$$\sum_{i=1}^{k}\left(\sum_{j=i}^{k}\frac{1}{j}\right)\frac{\nabla^i y_{n+1}}{i} = \left(\sum_{j=0}^{k}\frac{1}{j}\right)hf_{n+1} - \frac{h^2}{2}f'_{n+1}, \quad y''_n = f'(t_n, y(t_n)) = ff_{y_n} + f_{t_n}$$

by deriving a set of methods which are highly stable and suitable for the integration of stiff system in (1.1). This takes the general form

$$\sum_{j=0}^{k}\bar{\alpha}_j y_{n+j} = h\sum_{j=0}^{k+1}\bar{\beta}_j f_{n+j} + h^2\sum_{j=0}^{k+1}\bar{\gamma}_j f'_{n+j} \quad \bar{\alpha}_k = 1, \quad k \geq 1, \tag{1.3}$$

for a corrector method and the general second derivative linear multistep method

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\sum_{j=0}^{k}\beta_j f_{n+j} + h^2\sum_{j=0}^{k}\gamma_j f'_{n+j}, \quad \alpha_k = 1 \tag{1.4}$$

is used as the predictor method, where $\{\alpha_j\}_{j=0}^{k-1}$ and $\{\beta_j\}_{j=0}^{k-1}$ are determined such that (1.4) have appropriate order p. The procedure for computing methods of Cash [1] is as follows ;

(a) Compute $\bar{y}_{n+k}^{(n)}$ as the solution of the conventional linear k-step formula

$$y_{n+k} - h\beta f_{n+k} - h^2\gamma_k f'_{n+k} = \sum_{j=0}^{k-1}\left(-\alpha_j y_{n+j} + h\beta_j f_{n+j} + h^2\gamma_j f'_{n+j}\right).$$

(b) Compute $\bar{y}_{n+k+1}^{(n)}$as the solution of

$$y_{n+k+1} - h\beta f_{n+k+1} - h^2\gamma_k g_{n+k+1} = -\alpha_{k-1}\bar{y}_{n+k}^{(n)} + h\beta_{k-1}f\left(\bar{y}_{n+k}^{(n)}\right)$$
$$+h^2\gamma_{k-1}f'\left(\bar{y}_{n+k}^{(n)}\right) + \sum_{j=0}^{k-2}\left(-\alpha_j y_{n+j+1} + h\beta_j f_{n+j+1} + h^2\gamma_j f'_{n+j+1}\right).$$

(c) Compute y_{n+k} from (1.3).

The output y_{n+k} in the third step (c) is the numerical solution of (1.1) at t_{n+k} from the above method. The method is $zero-$stable for $k \leq 9$ and $zero-$unstable for $k \geq 10$. Furthermore, Cash [11] examined exponential fitting on multi-derivative methods for the solution of stiff problems in (1.1) . However, a different approach has been proposed by Amodio et al [12], Brugnano and Trigiante ([13, 14] and references therein) , where the continuous IVPs (1.1) is approximated by a means of discrete boundary value problems (BVPs) using a linear multistep boundary value method by fixing the initial $k_1(< k)$ number of solution values $(a1)$ and the last $k_2(= k - k_1)$ number of solution values $(a2)$ of the form,

$$\sum_{j=-k_1}^{k_2} \alpha_j y_{n+j} = h \sum_{j=-k_1}^{k_2} \beta_j f_{n+j}, \quad k_1, k_2 \in N, \quad k_1 + k_2 = k, \tag{1.5}$$

$$\underbrace{y_1, y_2, \cdots, y_{k_1-1}}_{\text{(a1)}} \qquad \underbrace{y_{k_1}, \cdots, y_{N-1}}_{\text{solution values to be generated by the BVM}} \qquad \underbrace{y_N, \cdots, y_{N+k_2-1}}_{\text{(a2)}}$$

Axelsson and Verwer [15], Ehigie et al [16], Jator and Sahi [17] also considered boundary value techniques on the IVPs (1.1). The BVM overcome the Dahlquist barrier theorem for LMMs in (1.2). Here k_1 is the number of roots lying inside a unit circle and k_2 is the number of roots lying outside the unit circle of the stability polynomial of the main method in (1.5) (see, Definition $(2.1 - 2.3)$). An Example of a BVM in (1.5) is the generalized BDF (GBDF)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h f_{n+u}; \quad k \geq 1, \tag{1.6}$$

as the main formula, while the initial and final conditions are obtained from fixing the solution values

$$y_1, y_2, \cdots, y_{k_1-1}, \quad y_N, \cdots, y_{N+k_2-1}.$$

This is a generalization of BDF in [2, page 246] as a BVM for numerical solution of (1.1) with $k_1 = u$ defined as

$$u = \begin{cases} \frac{k+2}{2}; & k \quad even \\ \frac{k+1}{2}; & k \quad odd \end{cases} \tag{1.7}$$

The method in (1.6) is $A_{u,k-u}-$stable (that is u is number of roots inside a unit circle while, $k - u$ is the number of roots lying outside the unit circle) , thus implemented with $(u, k - u)$-boundary conditions (see Definition $(2.1 - 2.3)$). BVMs have been effective in solving both initial and boundary value problems since they share special properties of both LMMs and RKMs such as good stability properties, high attainable order and effective for parallel computation of the solution of (1.1), see ([18, 19, 20, 21, 22, 23, 24, 25, 26, 27]), refer also to the monograph of [14]. The BVMs and block BVMs have been used to approximate the solution of delay differential equations [28, 29] and differential algebraic equations in [30]. Recently, [31, 32] studied Hamiltonian problems. Volterra integro-differential equations are investigated in [33, 34]. Moreso, neutral Pantograph equations and neutral multi-delay differential equations have been considered in [35, 36] using BVMs. In this article, we derive SDGEBDFs along with its initial methods and final methods which are of the same order. Thus, error of lower order during the integration process on the entire interval are avoided.

The paper is organized as follows. In Section 2, we recall the properties of second derivative boundary value methods (SDBVM) as well as its stability. In Section 3, is the construction of second derivative generalized extended backward differentiation formulas (SDGEBDFs) where the stability properties are discussed. Section 4 is on the effects of additional methods on SDGEBDFs during implementation. Numerical experiments are presented in Section 5. The conclusion of the article is in Section 6

2. THE SECOND DERIVATIVE BOUNDARY VALUE METHODS (SDBVM)

The IVPs in (1.1) can be approximated by the following second derivative k-step linear multistep formula

$$\sum_{j=-k_1}^{k_2} \alpha_j y_{n+j} = h \sum_{j=-k_1}^{k_2} \beta_j f_{n+j} + h^2 \sum_{j=-k_1}^{k_2} \gamma_j f'_{n+j}, \quad k_1, k_2 \in N, \quad k_1 + k_2 = k, \tag{2.1}$$
$$y_1, y_2, \cdots, y_{k_1-1}, \quad y_N, \cdots, y_{N+k_2-1},$$

of order p with k_1 initial conditions and k_2 final conditions at the boundary of interest (see [13, 14]). y_n is the discrete approximation of the solution $y(t_n)$, $t_n = t_0 + nh$ denotes the uniform point with equal spacing h, $h = \frac{(T-t_0)}{s}$, $s = N + k_2 - 1$, $f_n = f(t_n, y_n)$ and $f'_n = f'(t_n, y_n) = \frac{df(t_n,y_n)}{dt} \mid_{(t_n,y_n)}$. In order to implement (2.1) as a SDBVM, $k_1 - 1$ initial solution values $y_1, y_2, \cdots, y_{k_1-1}$ and k_2 final solution values $y_N, \cdots, y_{N+k_2-1}$ are needed, beside the initial value y_0 given by the continuous IVPs (1.1). These can be supplied by the following additional initial formulas

$$\sum_{i=0}^{k} \alpha_i^{(j)} y_i = h \sum_{i=0}^{k} \beta_i^{(j)} f_i + h^2 \sum_{j=0}^{k} \gamma_i^{(j)} f'_i; \quad j = 1(1)k_1 - 1, \tag{2.2}$$

and final additional formulas

$$\sum_{i=0}^{k} \alpha_{k-i}^{(j)} y_{N-i} = h \sum_{i=0}^{k} \beta_{k-i}^{(j)} f_{N-i} + h^2 \sum_{i=0}^{k} \gamma_{k-i}^{(j)} f'_{N-i}; \quad j = (N-k_2) + 1(1)N. \tag{2.3}$$

Here the composite scheme characterized by (2.1), (2.2) and (2.3) is a SDBVM assumed to have uniform order p. Thus, the method in (2.1) which is assumed to be $O_{k_1,k_2}-$stable, $A_{k_1,k_2}-$stable is used with $(k_1, k_2)-$boundary conditions. The composite SDBVM of (2.1, 2.2, 2.3) can be written in a composite matrix form as will be seen in section 3. That is, the stability polynomial of (2.1) has the root type distribution $(k_1, 0, k_2)$. To characterize the stability of the method to be considered, the notion of zero-stability ($O-$stability) and $A-$stability of SDLMMs from the theory of second derivative initial value methods (IVM) in (1.4) are readily generalized to SDBVM. Let

$$\rho(r) = \sum_{j=0}^{k} \alpha_j r^j, \quad \sigma(r) = \sum_{j=0}^{k} \beta_j r^j, \quad \varsigma(r) = \sum_{j=0}^{k} \gamma_j r^j, \tag{2.4}$$

be first, second and third characteristics polynomials associated with (1.4) respectively. Here,

$$\prod(R, z) = \rho(r) - z\sigma(r) - z^2\varsigma(r), \quad z = h\lambda \tag{2.5}$$

is the stability polynomial when (1.4) is applied on $y' = \lambda y$; $y'' = \lambda^2 y$, $Re(\lambda) < 0$. Then are the following definitions as in [13, 14] for (1.4).

Definition 2.1. *A polynomial $\rho(r)$ of degree $k = k_1 + k_2$ is an $S_{k_1,k_2}-$polynomial, if its roots $\{r_j\}_{j=1}^{k}$ are such that $|r_1| \leq |r_2| \leq \cdots |r_{k_1}| < 1 < |r_{k_1+1}| \leq \cdots \leq |r_k|$.*

Definition 2.2. *A polynomial $\rho(r)$ of degree $k = k_1 + k_2$ is an $N_{k_1,k_2}-$polynomial, if its roots $\{r_j\}_{j=1}^{k}$ are such that $|r_1| \leq |r_2| \leq \cdots |r_{k_1}| \leq 1 < |r_{k_1+1}| \leq \cdots \leq |r_k|$ with simple zeros of unit modulus.*

remark 2.1. *If $k_1 = k$, $k_2 = 0$, an $N_{k_1,k_2}-$polynomial reduces to a Von-Noumann polynomial and $S_{k_1,k_2}-$polynomial similarly reduces to a Schur-polynomial respectively as in the case of (1.4). In fact, A Linear multistep method in (1.2) is zero-stable (O-stability) if the corresponding polynomial $\rho(r)$ in (2.4) is an Von-Noumann polynomial and A-stable if the corresponding polynomial $\prod(r,z)$ in (2.5) is an Schur polynomial with $Re(z) < 0$.*

Definition 2.3. *A SDBVM (2.1) with $(k_1,k_2)-$boundary conditions where $k = k_1 + k_2$ is ;*

(a) *$O_{k_1,k_2}-$stable if the corresponding polynomial $\rho(r)$ in (2.4) is an $N_{k_1,k_2}-$polynomial.*
(b) *$(k_1,k_2)-$absolutely stable for a given $z \in \mathbb{C}$, if the polynomial $\prod(r,z)$ in (2.5) is an $S_{k_1,k_2}-$polynomial.*
(c) *Similarly, the region $D_{k_1,k_2} = \{z \in \mathbb{C} : \prod(r,z) \quad is \quad a \quad S_{k_1,k_2}-polynomial\}$ is said to be the region of $(k_1,k_2)-$absolute stability. Here $\prod(r,z)$ is a polynomial of type $(k_1,0,k_2)$.*
(d) *$A_{k_1,k_2}-$stable if $\mathbb{C}^- \subseteq D_{k_1,k_2}$.*

The following definition will be found useful.
A SDBVM is $A_{k_1,k_2}(\alpha)-$stable if the stability region is the wedge $W_\alpha = \{|\ arg(z) - \pi\ | \leq \alpha, \quad \alpha < \frac{\pi}{2}, \quad Re(z) < 0\}$.
Take note that $A_{k_1,k_2}-$ stability is equivalent to $A_{k_1,k_2}(\frac{\pi}{2})$ by this definition. Note further that the stability region of the methods considered in this paper are the exterior of the closed curves of the root loci of the stability polynomial of the methods. Examples of SDBVM (2.1) are the second derivative generalized backward differentiation formulas (SDGBDFs) [37]

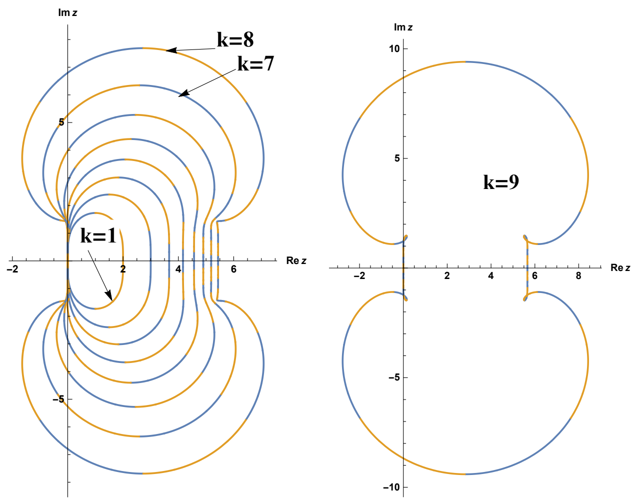
$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_u f_{n+u} + h^2 f'_{n+u}, \quad \forall \quad k \geq 1, \tag{2.6}$$

and

$$y_{n+u} - y_{n+u-1} = h\sum_{j=0}^{k} \beta_j f_{n+j} + h^2 \sum_{j=0}^{k} \gamma_j f'_{n+j} \forall \quad k \geq 1,$$

is the second derivative generalized Adam methods (SDGAMs) in [38] used as the main methods with u given as in (1.7), while the initials and final conditions are second derivative linear multistep formulas (SDLMFs) obtained by fixing the solution values

$$y_1, y_2, \cdots, y_{k_1-1}, \quad y_N, \cdots, y_{N+k_2-1}.$$



(A) (B)

Figure 1: Boundary loci of the SDBDF (3.1) of order $p = k+1$, (A) $k = 1(1)8$ and (B) $k = 9$

3. SECOND DERIVATIVE GENERALIZED EXTENDED BACKWARD DIFFERENTIATION FORMULAS (SDGEBDFS)

The common family of second derivative linear multistep formulas widely used in the solution of (1.1) is the conventional second derivative backward differentiation formulas (SDBDF) defined by

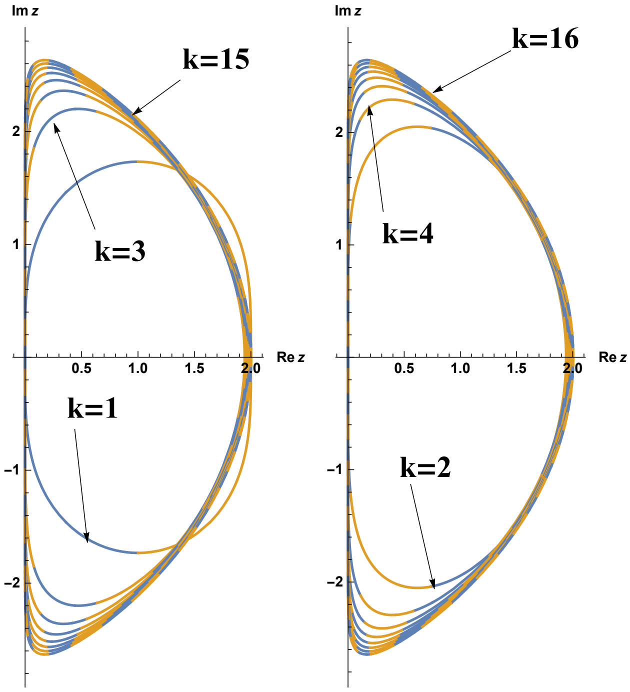
$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h f_{n+k} - \frac{h^2}{2} f'_{n+k}, \quad \forall \quad k \geq 1, \tag{3.1}$$

with order $p = k + 1$ which employs the second derivative $y''_n = f'(t_n, y(t_n)) = f f_{y_n} + f_{t_n}$ of (1.1). The method in (3.1) is A-stable for $k \leq 2$, $A(\alpha)$-stable for $k \leq 8$ and unstable for $k \geq 9$ (its boundary loci are shown in Fig. 1). Our purpose is to derive A_{k_1,k_2}-stable formulas that satisfy stability at infinity and higher order for any step number of $k \geq 1$ from (1.4) or (2.1). In this regard, the SDBVM of interest herein is

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=k}^{2k-1} \beta_j f_{n+j} + h^2 f'_{n+k}, \quad \forall \quad k \geq 1, \tag{3.2}$$

$$\underbrace{y_1, \cdots, y_{k-1}}_{\text{(a)}} \qquad \underbrace{y_k, \cdots, y_{N-1}}_{\text{solution values to be generated by the SDBVM}} \qquad \underbrace{y_N, \cdots, y_{N+k-2}}_{\text{(b)}}$$

to be used as the main formula, while the the solution output (a) and (b) are to be provided or replaced by SDLMF equations at the points $t_{n+1}, \cdots, t_{n+k-1}$ and $t_{n+N}, t_{n+N+1}, \cdots, t_{n+N+k-2}$. Thus for $k = 1$ in (3.2) is the conventional SDBDF in (3.1). Notice that (3.2) is in the



(A) (B)

Figure 2: Boundary loci of the SDGEBDFs (3.2) of order $p = 2k$, (A) $k = 1(1)16$ and (B) $k = 2(2)16$

sense of (1.5) of Cash (1981) in [1]. The $2k+1$ parameters allow the construction of methods in (3.2) of maximal order $p = 2k$. For each $k > 1$, the method in (3.2) must be used with $(k, k-1)$ $-$boundary conditions since it is found to be $0_{k,k-1}-$stable and $A_{k,k-1}-$stable method. By this the method in (3.2) has k number of roots inside the unit circle and $k-1$ number of roots outside the unit circle. The method in (3.2) shall be referred to as second derivative generalized extended backward differentiation formulas (SDGEBDFs) with $(k-1)$ future points at $\{t_{n+j}\}_{j=k+1}^{2k-1}$ and the corresponding future solution are $\{y_{n+j}\}_{j=k+1}^{2k-1}$. The points $\{t_{n+j}, y_{n+j}\}_{j=k+1}^{2k-1}$ are also referred to as super-future points [2, page 267] . From the method in (3.2),

$$\sum_{j=0}^{k} \alpha_j y\left(t_n + jh\right) - h \sum_{j=k}^{2k-1} \beta_j y'\left(t_n + jh\right) - h^2 y''\left(t_n + kh\right) = C_{2k+1} h^{2k+1} y^{(2k+1)}\left(t_n\right) + O\left(h^{2k+2}\right). \quad (3.3)$$

By expanding (3.2) in terms of Taylor series and using the method of undetermined coefficients (3.3) results into a system of linear equations for the coefficients $\{\alpha_j\}$, and $\{\beta_j\}$ given in Tables 3 and 4.

3.1. **The consistency, order and stability of SDGEBDFs.** Following [5, 39], we define the linear difference operator $L[y(t), h]$ from (3.3) associated with SDGEBDFs in (3.2) as

$$L\left[y\left(t_n\right), h\right]=\sum_{j=0}^{k} \alpha_j y\left(t_n+j h\right)-h \sum_{j=k}^{2k-1} \beta_j y^{\prime}\left(t_n+j h\right)-h^2 y^{\prime\prime}\left(t_n+k h\right), \tag{3.4}$$

where $y\left(t_n\right)$ is a sufficiently differentiable function as in (3.3). The (3.4) results into local truncation error (*lte*) of the SDGEBDFs (3.2), since $y\left(t_n\right)$ is assumed exact solution of (1.1). We can expand the terms in (3.4) as a Taylor series about the point t_n to obtain the expression,

$$L\left[y\left(t_n\right), h\right]=C_0 y\left(t_n\right)+C_1 h y^{\prime}\left(t_n\right)+\cdots+C_p h^p y^{(p)}\left(t_n\right)+C_{p+1} h^{p+1} y^{(p+1)}\left(t_n\right)+\cdots,$$

where

$$\left.\begin{array}{l} C_0=\sum_{j=0}^{k} \alpha_j \quad C_1=\sum_{j=0}^{k} j \alpha_j-\sum_{j=k}^{2k-1} \beta_j \quad C_2=\sum_{j=0}^{k} \frac{j^2}{2!} \alpha_j-\sum_{j=k}^{2k-1} j \beta_j-1, \quad \cdots \\ \qquad C_p=\sum_{j=0}^{k} \frac{j^p}{p!} \alpha_j-\sum_{j=k}^{2k-1} \frac{j^{p-1}}{(p-1)!} \beta_j-\frac{k^{p-2}}{(p-2)!} \quad p \geq 1, \quad k>2 \end{array}\right\}. \tag{3.5}$$

The $C_{p+1} \neq 0$ is the error constant. The order conditions defined by (3.5) for the constants $\{\alpha_j\}_{j=0}^{k}, \{\beta_j\}_{j=k}^{2k}$ is equivalent to

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 2 & \cdots & k & 1 & 1 & \cdots & 1 \\ 0 & 1^2 & 2^2 & \cdots & (k)^2 & 2.(k) & 2.(k+1) & \cdots & 2.(2k-1) \\ \vdots & & & & & & & & \vdots \\ \vdots & & & & & & & & \vdots \\ 0 & 1^p & 2^p & \cdots & (k)^p & p.k & p.(k+1)^{p-1} & \cdots & p.(2k-1)^{p-1} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_{k-1} \\ -\beta_k \\ \vdots \\ -\beta_{2k-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2 \\ \vdots \\ \vdots \\ p(p-1)k^{p-2} \end{pmatrix};$$

with the assumption that the method is of order p with $C_{p+1} \neq 0$. The method coefficients $\{\alpha_j\}_{j=0}^{k}, \{\beta_j\}_{j=k}^{2k}$ are in Tables 3 and 4. The following definitions becomes obvious.
The SDGEBDFs (3.2) is of order p, if

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

where $C_{p+1} \neq 0$ is the error constant (EC) and its principal local truncation error (lte) is given as

$$lte=C_{p+1} h^{p+1} y^{(p+1)}\left(t_n\right)+O\left(h^{p+2}\right), \quad C_{p+1} \neq 0$$
$$C_{p+1}=\sum_{j=0}^{k} \frac{j^{p+1}}{(p+1)!} \alpha_j-\sum_{j=k}^{2k-1} \frac{j^p}{p!} \beta_j-\frac{k^{p-1}}{(p-1)!}.$$

The SDGEBDFs in (3.2) is consistent if, it has an order $p \geq 1$. Now, we analyze the stability of the proposed method (3.2) , (see, [2]), by applying (3.2) on the test problem

$$y^{\prime}=\lambda y, \quad , \quad Re(\lambda)<0, \tag{3.6}$$

Take note that application of differentiation on (3.11) gives $y'' = \lambda^2 y$ to yield the characteristic stability polynomial

$$\prod (r,z) = \rho\,(r) - z\sigma\,(r) - z^2 \varsigma(r) = \sum_{j=0}^{k} \alpha_j r^j - z \sum_{j=k}^{2k-1} \beta_j r^j - z^2 r^k, \quad z = \lambda h, \quad Re(z) < 0, \tag{3.7}$$

used to determine its boundary locus of z. Giving $r = e^{i\theta}$, we obtain two roots of $\prod(r,z)$ with respect to z for any value of k in (3.2) (where (3.7) is a quadratic equation in z) to give the stability regions defined by z. This is given in Fig. 2 for odd and even values of k respectively. The root distribution of this polynomial (3.7) remains the same $(k_1, 0, k_2)$ as z varies in $\mathbb{C}^-$ if it is $A_{k_1,k_2}-$stable. Theorem 4.7.1 and 4.11.1 in [14] applies in the case of SDGEBDFs in (3.2), here $k_1 = k$, $k_2 = k-1$ in (3.2). The discrete problem generated by the $(2k)-$step SDGEBDFs (3.2) with $(k, k-1)$-boundary conditions can be written in compact form,

$$AY - hBF - h^2 IF' = - \begin{pmatrix} \sum_{j=0}^{k-1} \alpha_j y_{n+j} \\ \vdots \\ \alpha_j y_n \\ 0 \\ \vdots \\ 0 \\ -h\beta_k f_N \\ \vdots \\ -h \sum_{j=0}^{k-1} \beta_{k+j} f_{N-1+j} \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{3.8}$$

where

$$A=\begin{pmatrix} \alpha_k & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & & & & \vdots \\ \alpha_0 & & \ddots & \ddots & & & \vdots \\ 0 & \alpha_0 & & \alpha_k & 0 & & \vdots \\ \vdots & \ddots & \ddots & & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & \alpha_0 & \cdots & \alpha_k \end{pmatrix}_{(N-k)\times(N-k)}, B=\begin{pmatrix} \beta_k & \cdots & \beta_{2k-1} & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \beta_k & \ddots & \ddots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & \beta_{2k-1} \\ \vdots & & & & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & \beta_k \end{pmatrix}$$

The A, B and I (Identity matrix) are Toeplitz matrices (T-matrices) of the same dimension and

$$Y=(y_k,y_{k-1},\cdots,y_{N-1})^T, \quad F=(f_k,f_{k-1},\cdots,f_{N-1})^T, \quad F'=\left(f'_k,f'_{k-1},\cdots,f'_{N-1}\right)^T,$$

are the solution, function and derivative function vectors (3.8). The coefficient matrices A, B in (3.8) are T-matrices having lower band with k (number of initial conditions) upper band with $t=k-1$ (number of final conditions). Since y_0 is provided by the continuous problem (1.1), the $k-1$ extra initial solution values $y_1,\ldots,y_{k-1}$ in (3.2) are given by the initial methods

$$\sum_{i=0}^{2k-1}\alpha_i^{(j)}y_j=h\beta_i^{(j)}f_j+h^2\gamma_i^{(j)}f'_j; \quad j=1(1)k-1, \quad k\geq 2, \tag{3.9}$$

and the $k-1$ extra final solution values $y_N,y_{N+1},\cdots,y_{N+k-1}$ are given by the final methods,

$$\sum_{i=0}^{2k-1}\alpha_i^{(j)}y_{N-k-1+i}=h\beta_i^{(j)}f_{N-k-1+j}+h^2\gamma_i^{(j)}f'_{N-k-1+j}; \quad j=k+1(1)2k-1, \quad k\geq 2, \tag{3.10}$$

preferably of uniform order. The composite scheme of (3.2), (3.9), (3.10) is a SDBVM assumed therefore to have uniform order. The composite SDBVM with (3.2) as the main method, (3.9) as the initial method and (3.10) as the final method can now be written in a compact form,

$$\bar{A}Y-h\bar{B}F-h^2\bar{C}F'=0, \quad 0=(0,0,\cdots,0)^T, \tag{3.11}$$

where $\bar{A} = [a \mid A_s] \in R^{(s)\times(s+1)}$ is given by

$$\bar{A} = [a \mid A_s]$$

$$= \left(\begin{array}{c|cccccccccc}
\alpha_0^{(1)} & \alpha_1^{(1)} & \cdots & \alpha_k^{(1)} & \alpha_{k+1}^{(1)} & \cdots & \alpha_{2k-1}^{(1)} & 0 & 0 & 0 & 0 \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & & & & \vdots \\
\alpha_0^{(k-1)} & \alpha_1^{(k-1)} & \cdots & \alpha_k^{(k-1)} & \alpha_{k+1}^{(k-1)} & \cdots & \alpha_{2k-1}^{(k-1)} & 0 & & & \vdots \\
\alpha_0 & \alpha_1 & \cdots & \alpha_k & 0 & \cdots & \cdots & 0 & & & 0 \\
0 & \ddots & \ddots & & \ddots & \ddots & & & & & \vdots \\
\vdots & 0 & \ddots & \ddots & & \ddots & \ddots & & & & \vdots \\
\vdots & 0 & 0 & \ddots & \ddots & & \ddots & \ddots & & & \vdots \\
\vdots & 0 & \cdots & 0 & \alpha_0 & \alpha_1 & \cdots & \alpha_k & 0 & \cdots & 0 \\
\vdots & 0 & \cdots & 0 & \alpha_0^{(k+1)} & \alpha_1^{(k+1)} & \cdots & \alpha_k^{(k+1)} & \alpha_{k+1}^{(k+1)} & \cdots & \alpha_{2k-1}^{(k+1)} \\
\vdots & & & & \vdots & \vdots & & \vdots & \vdots & \vdots & \\
0 & 0 & \cdots & 0 & \alpha_0^{(2k-1)} & \alpha_1^{(2k-1)} & \cdots & \alpha_k^{(2k-1)} & \alpha_{k+1}^{(2k-1)} & \cdots & \alpha_{2k-1}^{(2k-1)}
\end{array}\right)$$

and $\bar{B} = [b \mid B_s] \in R^{(s)\times(s+1)}$ is similarly given by

$$\bar{B} = [b \mid B_s] = \left(\begin{array}{c|cccccccccc}
 & \beta_1^{(1)} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & & \cdots & 0 \\
 & 0 & \beta_2^{(2)} & \ddots & & & & & & & \vdots \\
 & \vdots & \ddots & \ddots & \ddots & & & & & & \vdots \\
 & \vdots & & 0 & \beta_{k-1}^{(k-1)} & 0 & \cdots & \cdots & & & 0 \\
 & \vdots & & & 0 & \beta_k & \beta_{k+1} & \cdots & \beta_{2k-1} & 0 & 0 \\
 & \vdots & & & & \ddots & \ddots & \ddots & \cdots & \ddots & 0 \\
0 & \vdots & & & & & \ddots & \beta_k & \beta_{k+1} & \cdots & \beta_{2k-1} \\
 & \vdots & & & & & & 0 & \beta_{k+1}^{(k+1)} & 0 & 0 \\
 & \vdots & & & & & & & 0 & \ddots & 0 \\
 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & & \cdots & 0 & \beta_{2k-1}^{(2k-1)}
\end{array}\right)$$

$$\bar{C} = [c \mid C_s] = \left(\begin{array}{c|cccccccccc} & \gamma_1^{(1)} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & & \cdots & 0 \\ & 0 & \gamma_2^{(2)} & \ddots & & & & & & & \vdots \\ & \vdots & \ddots & \ddots & \ddots & & & & & & \vdots \\ & \vdots & & 0 & \gamma_{k-1}^{(k-1)} & 0 & \cdots & \cdots & & & 0 \\ & \vdots & & & 0 & \gamma_k & 0 & \cdots & & 0 & 0 \\ & \vdots & & & & \ddots & \ddots & \ddots & \cdots & \ddots & 0 \\ 0 & \vdots & & & & & \ddots & \gamma_k & 0 & \cdots & 0 \\ & \vdots & & & & & 0 & 0 & \gamma_{k+1}^{(k+1)} & 0 & 0 \\ & \vdots & & & & & & & 0 & \ddots & 0 \\ & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & & \cdots & 0 & \gamma_{2k-1}^{(2k-1)} \end{array} \right); \quad \gamma_k = 1$$

In this way, we solve the non-linear algebraic system (3.11) to obtain the vector Y of solution values of $(1.1))$. The matrix $\bar{A} - z\bar{B} - z^2\bar{C}$, has a quasi-Toeplitz structure see [26, 40, 41] as a result of the additional formulas from (3.9) and (3.10). The (3.11) is therefore equivalent to the one-block method,

$$A_s Y_{n+1} + A_0 Y_n = h\left(B_s F_{n+1} + B_0 F_n\right) + h^2\left(C_s F'_{n+1} + C_0 F'_n\right), \tag{3.12}$$

where

$$A_0 = (0 \mid a) = \left(\begin{array}{c|c} & \alpha_0^{(1)} \\ & \vdots \\ & \alpha_0^{(k-1)} \\ 0_{(s)\times(s-1)} & \alpha_0 \\ 0 & \vdots \\ & 0 \\ & \vdots \\ & 0 \end{array} \right), \quad B_0 = (0 \mid b) = \left(\begin{array}{c|c} & 0 \\ & \vdots \\ 0_{(s)\times(s-1)} & 0 \\ & \vdots \\ & 0 \end{array} \right)$$

and

$$\begin{aligned} B_0 = C_0; \quad -A_s^{-1}A_0 = [0 \mid e]; \quad e = (1, 1, \cdots, 1)^T \\ Y_{n+1} = \left(y_{n+1}, y_{n+2}, \cdots, y_{n+s}\right)^T, \quad Y_n = \left(y_{n-s+1}, y_{n-s+2}, \cdots, y_n\right)^T \\ F_{n+1} = \left(f_{n+1}, f_{n+2}, \cdots, f_{n+s}\right)^T, \quad F_n = \left(f_{n-s+1}, f_{n-s+2}, \cdots, f_n\right)^T \\ F'_{n+1} = \left(f'_{n+1}, f'_{n+2}, \cdots, f'_{n+s}\right)^T, \quad F'_n = \left(f'_{n-s+1}, f'_{n-s+2}, \cdots, f'_n\right)^T. \end{aligned} \tag{3.13}$$

The challenge of resolving implicitness that arise when implementing LMM (1.2) and SDLMM (3.1) in a step-by-step procedure (1.1) is easily removed by the SDBVM (3.2) since

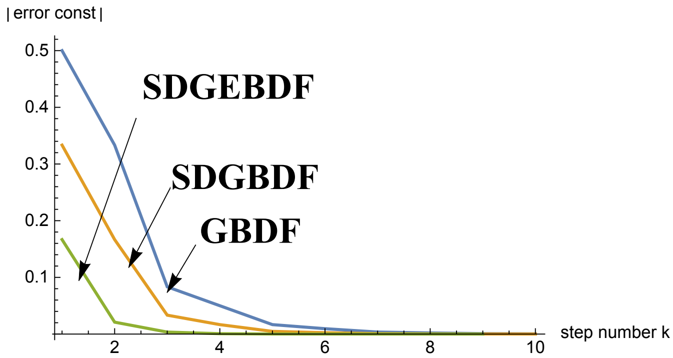


Figure 3: The plot of | $error\ constants$ | against step number k of the GBDF in (1.5), SDGBDF in (2.6) and SDGEBDF in (3.2)

the block method in (3.12) can be made self starting. The resolution of implicitness in the LMM (1.2) and SDLMM (3.1) is usually done by Newton-Raphson iterative process which requires for fast convergence, computing an exact jacobian may be quite demanding when the function $f(t, y)$ is complicated. Generally, step rejection do arise in the case of implementing the LMM (1.2) and SDLMM (3.1) when the accuracy of the generated solution fall short of the accuracy demanded by the user. In fact, this increases the number of functions evaluations on implementation of the LMM (1.2) and SDLMM (3.1), which is a challenge when the ODE (1.1) is very stiff. Whereas, a SDBVM compute its solution of an IVP (1.1) in a block Y arising from solving the system of non-linear equation (3.8) . The block size of Y is determined by the root distribution of the stability polynomial (3.7) of the main method in (3.2) and the number of times $(N-k_1)$ we need to shift the main method to obtain the other equations and in general the $s = N + k_2 - 1$ is such that $s > k$ the step number of the linear multistep formula of the main method (3.2) of the SDBVM. The k_1 and k_2 defines the root distribution $(k_1, 0, k_2)$ of the stability polynomial of the main method (3.2) in the SDBVM. The step size may be choosen as $h = \frac{t_0 - T}{s} > 0$ such that $0 < h < 1$. The number of functions evaluation in a SDBVM is directly proportional to s which is the dimension of the function block F in (3.13) for a given step number k. We have achieved high accuracy with the proposed SBBVM (3.2) reported in later sections, at relatively smaller N when compared to some other existing methods, see for examples Tables $(5, 6, 7, 8, 9)$. A consistent SDGEBDFs in (3.2) is correctly used with $z \in \mathbb{C}^-$, where its stability polynomial $\prod(r, z)$ in (3.7) is of the type $(k, 0, k-1)$, if k conditions are imposed at the initial points and $k-1$ conditions imposed at the boundary of the interval of interest of the integration. That is, for a given SDGEBDFs (3.2) with $(k, k-1)$ $-$boundary conditions, the corresponding family of matrices $T_N^{(k)} = A - zB - z^2C$ from (3.8) are well conditioned when $z \in D_{k,k-1}$ ($D_{k,k-1}$ is D_{k_1,k_2} in definition $(2.3d)$). This means as well that the condition number of $T_N^{(k)}$ are uniformly bounded with respect to increasing N and a varying k,in fact, the necessary condition for having method (3.11) well-conditioned is to have its eigenvalues bounded away from zero and infinity, as N increases, see Table 2. Note that k

is the number of roots inside the unit circle and $k-1$ is the number of roots outside of (3.7). Here the characteristics polynomial of SDGEBDFs (3.2) in (3.7) is an $S_{k,k-1}-$ polynomial thus SDGEBDFs (3.2) is implemented as SDBVM with $(k,k-1)-$boundary condition. By comparing with second derivative generalized backward differentiation formula in [37], the method in (3.2) are found to have higher order $p=2k$ and smaller error constants for the same value of the step number k (See, Fig. 3). Consider as an example the sixth order SDGEBDFs (3.2),

$$\begin{aligned} \frac{1402}{132165}y_n - \frac{1121}{9790}y_{n+1} + \frac{4138}{4895}y_{n+2} - \frac{195989}{264330}y_{n+3} = -\frac{24064 f_{n+3}}{44055}h \\ -\frac{548 f_{n+4}}{4895}h + \frac{49 f_{n+5}}{4895}h + \frac{1}{3}h^2 f'_{n+3}; \quad n = 0(1)N-4, \end{aligned} \tag{3.14}$$

which is $A_{3,2}-$stable and applied on (1.1) with two initial conditions

$$\begin{aligned} \frac{72}{1295}y_0 - \frac{1}{2}y_1 + \frac{144}{259}y_2 - \frac{36}{259}y_3 + \frac{8}{259}y_4 - \frac{9}{2590}y_5 = \frac{78}{259}hf_1 + \frac{36}{259}h^2 f'_1, \\ -\frac{9}{980}y_0 + \frac{9}{49}y_1 - \frac{1}{2}y_2 + \frac{18}{49}y_3 - \frac{9}{196}y_4 + \frac{1}{245}y_5 = \frac{6}{49}hf_2 + \frac{9}{49}h^2 f'_2, \end{aligned} \tag{3.15}$$

and two final conditions

$$\begin{aligned} -\frac{1}{320}y_{N-4} + \frac{1}{36}y_{N-3} - \frac{1}{8}y_{N-2} + \frac{1}{2}y_{N-1} - \frac{259}{576}y_N + \frac{1}{20}y_{N+1} = -\frac{13}{48}hf_N + \frac{1}{8}h^2 f'_N, \\ +\frac{72}{12019}y_{N-4} - \frac{1125}{24038}y_{N-3} + \frac{2000}{12019}y_{N-2} - \frac{4500}{12019}y_{N-1} + \frac{9000}{12019}y_N \\ -\frac{1}{2}y_{N+1} = -\frac{4110}{12019}hf_{N+1} + \frac{900}{12019}h^2 f'_{N+1}, \end{aligned} \tag{3.16}$$

which in one-block form as in (3.12),

$$A_s = \begin{pmatrix} \frac{-1}{2} & \frac{144}{259} & \frac{-36}{259} & \frac{8}{259} & \frac{-9}{25900} & 0 & \cdots & \cdots & 0 \\ \frac{9}{49} & \frac{-1}{2} & \frac{18}{49} & \frac{-9}{196} & \frac{1}{245} & 0 & \cdots & \cdots & 0 \\ \frac{-1121}{9790} & \frac{4138}{4895} & \frac{-195989}{264330} & 0 & 0 & 0 & \cdots & \cdots & 0 \\ \frac{1402}{132165} & \frac{-1121}{9790} & \frac{4138}{4895} & \frac{-195989}{264330} & 0 & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \frac{1402}{132165} & \frac{-1121}{9790} & \frac{4138}{4895} & \frac{-195989}{264330} & 0 & 0 \\ 0 & \cdots & 0 & \frac{-1}{320} & \frac{1}{36} & \frac{-1}{8} & \frac{1}{2} & \frac{-259}{574} & \frac{1}{20} \\ 0 & \cdots & 0 & \frac{72}{12019} & \frac{-1125}{24038} & \frac{2000}{12019} & \frac{-4500}{12019} & \frac{9000}{12019} & \frac{-1}{2} \end{pmatrix}_{s\times s}$$

$$B_s = \begin{pmatrix} \frac{78}{259} & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & \frac{6}{49} & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \frac{-24063}{44055} & \frac{-548}{4895} & \frac{49}{4895} & 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & \frac{-24063}{44055} & \frac{-548}{4895} & \frac{49}{4895} \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 & \frac{-13}{48} & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 & 0 & \frac{-4110}{12019} \end{pmatrix}_{s\times s}, B_0 = C_0 = \begin{pmatrix} 0_{(s\times s)} \end{pmatrix}$$

$$C_s = \begin{pmatrix} \frac{36}{259} & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & \frac{9}{49} & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 & \frac{1}{8} & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 & 0 & \frac{900}{12019} \end{pmatrix}_{s\times s}, A_0 = \left(\begin{array}{c|c} & \frac{72}{1290} \\ & \frac{-1}{9} \\ & \frac{1402}{132165} \\ 0_{(s-1)\times(s)} & 0 \\ & \vdots \\ & 0 \\ & \vdots \\ & 0 \end{array}\right) \tag{3.17}$$

4. EFFECTS OF ADDITIONAL METHODS ON THE STABILITY AND MINIMUM BLOCK SIZE IMPLEMENTATION OF THE BVMS SDGEBDFS

Generating the exact k initial and $k-1$ final values in the implementation of (3.2) on (1.1) may not be simple, especially with a high step number k of the main method (3.2). The alternative therefore, is to replace them by an equivalent number of equations formed by SDLMFs as in (3.9) and (3.10) preferably of the same order as in the example of (3.17). The introduction of the initial and final methods into a SDBVM implementation in (3.11) affects its stability. This stability is reduced to $A_{k_1,k_2}(\alpha)-$stability when these values are instead replaced by initial and final methods. To study this effect of the initial methods (3.9) and the final methods (3.10) on the whole composite schemes of the SDBVM, we obtain the following discrete problem

$$\left(A_s - zB_s - z^2C_s\right) y = -\left(A_0 - zB_0 - z^2C_0\right) y_0, \quad z = h\lambda, \tag{4.1}$$

in (3.12) (see, (3.6) and (3.7)). Here, $y = Y_{n+1}$ and $y_0 = Y_n$. The method in (4.1) will have a solution for all $Re(z) < 0$, if the eigenvalue of the matrix pencil

$$\left(A_s - \mu B_s - \mu^2 C_s\right), \tag{4.2}$$

have a positive real part for all values of the block size s and the method (4.1) is pre-stable likewise, that is

$$-A_s^{-1}a = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in R^s.$$

The matrix pencil in (4.2) is a Toeplitz matrix, if the main method (3.2) is being written in the compact form in (3.8) with $N > (k_1 + k_2)$. Thus, Theorem 5 in [14] is applicable on the methods. To implement the composite schemes(comprises of the main method (3.2), the initial methods (3.9) and the final methods (3.10)), some eigenvalue of the matrix pencil (4.2) may enter $\mathbb{C}^-$ for $k \geq 3$, as a result of extra rows introduced at the top and bottom in equation (3.12) respectively by the initial and final methods, see Fig. 4 . By this, the method becomes $A_{k_1,k_2}(\alpha)$-stable, the method (3.12) can be safely used for all the values of k in (3.2) for any particular problem provided that $z = h\lambda$ is not closed to imaginary axis. Nevertheless, Brugnano and Trigiante [14] introduced a slight modification to avoid the presences of eigenvalues of (4.2) in $\mathbb{C}^-$ on the composite schemes (3.12), by taking the output inside each block Y in (3.13) not uniformly spaced. For example, let

$$t_0, t_1, \cdots, t_r, t_{r+1}, \cdots, t_{s-r-1}, t_{s-r}, \cdots, t_{s-1}, t_s, \tag{4.3}$$

be the grid points inside the complete block Y and let the following output points

$$t_0, t_r, \cdots, t_{s-r}, t_s,$$

be equally spaced with steps size h. The remaining points in (4.3) are computed from

$$t_i = t_{i-1} + \nu^{r+1-i}h, \quad i = 1, \cdots, r, \tag{4.4}$$

$$t_{s-i} = t_{s+i-1} - \nu^{r+1-i}h, \quad i = 1, \cdots, r, \tag{4.5}$$

such that when $r = 1$, $\nu = 1$; when $r = 2$, $\nu = \frac{-1}{2} + \frac{\sqrt{5}}{2}$ and when $r = 3$, $\nu = 0.543689$. Thus, for the case $r \geq 4$, ν is determined from

$$\sum_{i=0}^{r} \nu^i - 1 = 0; \quad 0 < \nu \leq 1.$$

The points (4.4) and (4.5) are referred to as the initial and final auxiliary points, respectively. Table 1 shows the minimum value of r required for all the eigenvalues of the corresponding pencil (4.2) to have positive real part for all chosen values of s. s denote the block size of the method (3.12) and the matrix in (4.2), where the minimum value s^* $(s^* \leq s)$ to have an $A-$stable method may be different, depending on the step number k of main method and on the number r of the auxiliary grid points used. Thus, we have

$$y_s = -E_s^T \left(A_s - zB_s - z^2C_s\right)^{-1} \left(A_0 - zB_0 - z^2C_0\right) y_0 \equiv \phi(z)y_0,$$

from (4.1), where $E_s^T = (0, 0, ..., 0, 1) \in R^s$. The function $\phi(z)$ is analytical for $z \in \mathbb{C}^-$, since r auxiliary grid points are introduced, the matrix pencil in (4.2) contains all the eigenvalues

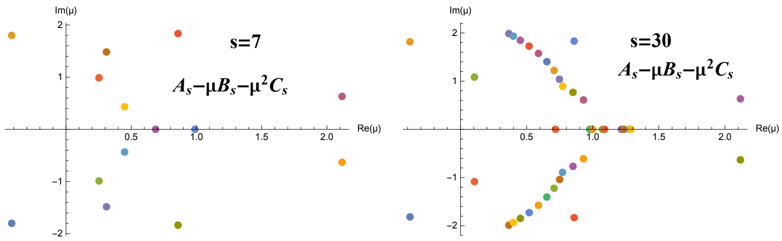


Figure 4: Eigenvalues of the pencil (4.2) corresponding to the sixth order SDGEBDFs (3.2) $(k = 3)$ for $s = 7, 30$.

with positive real part. Therefore,such methods are $A-$stable provided that

$$| \phi(it) | \leq 1 \quad \forall \quad t \in R \quad i = \sqrt{-1}.$$

Table 1 shows the values of s^* corresponding to different values of the number of r of auxiliary grid points used. It is clear that the larger r, the smaller the minimum blocksize s^* for a given step number k.

TABLE 1. Minimum blocksize s^* for $A-$stability

Boundary value methods												
GBDF [18] (order $p = k$)	k	1	2	3		4		5	6		7	
	r	1	1	1	2	1	2	2	2	3	1	2
	s^*	1	2	7	4	19	6	6	8	7	12	7
SDGEBDFs (order $p = 2k-1$)	k	1	2	3		4		5	6			
	r	1	1	2		4		4	8			
	s^*	2	3	5		7		9	11			

TABLE 2. Condition number of the matrix $A - zB - z^2C$ associated with $(A_{k,k-1})$ −stable SDGEBDFs (3.2); $h = 1$; $z = h\lambda$, $m = 1$

λ			1					-1		
$N \setminus k$	2	3	4	5	6	2	3	4	5	6
50	4.48	5.13	5.51	5.78	5.98	2.43	2.51	2.57	2.61	2.65
100	4.50	5.14	5.53	5.79	5.99	2.44	2.51	2.57	2.62	2.65
500	4.50	5.15	5.53	5.80	6.00	2.44	2.52	2.57	2.62	2.66
1000	4.50	5.15	5.53	5.80	6.00	2.44	2.52	2.57	2.62	2.66
5000	4.50	5.15	5.53	5.80	6.00	2.44	2.52	2.57	2.62	2.66

TABLE 3. The coefficients, order p and error constants C_{p+1} of SDGEBDFs (3.2)

k	α_0	α_1	α_2	α_3	α_4	α_5	β_k
1	2	-2	0	0	0	0	-2
2	$\frac{-7}{34}$	$\frac{40}{17}$	$\frac{-73}{34}$	0	0	0	$\frac{-29}{17}$
3	$\frac{1402}{44055}$	$\frac{-3363}{9790}$	$\frac{12414}{4895}$	$-\frac{195989}{88110}$	0	0	$-\frac{24064}{14685}$
4	$-\frac{1065089}{185950008}$	$\frac{1600568}{23243751}$	$-\frac{1136538}{2582639}$	$\frac{61590472}{232343751}$	$-\frac{4226322495}{185950008}$	0	$\frac{300316524}{422632495}$
5	$\frac{16732394834}{14990986666675}$	$-\frac{219331441565}{14391347200008}$	$\frac{1869862440}{179891840000}$	$-\frac{306604587530}{594639466667}$	$\frac{4907291636530}{1798918900001}$	$-\frac{829806438712891}{359753680000200}$	$-\frac{14438494722877}{8994592000005}$

TABLE 4. (continuation) The coefficients, order p and error constants C_{p+1} of SDGEBDFs (3.2)

k	β_{k+1}	β_{k+2}	β_{k+3}	β_{k+4}	p	C_{p+1}
1	0	0	0	0	2	$\frac{1}{6}$
2	$-\frac{4}{17}$	0	0	0	4	$-\frac{23}{1095}$
3	$-\frac{1644}{4895}$	$\frac{147}{4895}$	0	0	6	$\frac{24027}{6859615}$
4	$\frac{72595008}{422632495}$	$-\frac{10642704}{422632495}$	$\frac{946752}{422632495}$	0	8	$-\frac{29113654}{44376411975}$
5	$-\frac{254369092080}{599639466667}$	$\frac{47357245180}{599639466667}$	$-\frac{21931447960}{1798918400001}$	$\frac{1159678965}{1199278933334}$	10	$\frac{25116126583340}{191685287342677821}$

5. Numerical experiments

In this section, we report some numerical results using MATLAB 2010a to examine the accuracy of the methods (3.2) on some stiff problems. The arising SDGEBDFs (3.14) for $k=3$, $p=6$ is implemented in one-block form (3.12) along with two initial methods and two final methods in (3.15) and (3.16) respectively. Here the one-block form is denoted by SDGEBDFs3.

Problem 1: Consider the linear problem in [14, 17]

$$y' = \begin{pmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix};$$

$$y(t) = \frac{1}{2} \begin{pmatrix} e^{-2t} + e^{-40t}\left(cos(40t) + sin(40t)\right) \\ e^{-2t} - e^{-40t}\left(cos(40t) + sin(40t)\right) \\ 2e^{-40t}\left(cos(40t) - sin(40t)\right) \end{pmatrix}$$

Table 5 contains the maximum relative error $\max\left(\mid y - y(t) \mid /(1+ \mid y(t) \mid)\right)$ in the interval $0 \leq t \leq 1$ using SDGEBDFs3. It is seen from the numerical results in Table 5 that the SDGEBDFs3 performance better when compared with Adams-type second derivative methods (SDAM) of order $p=6$ in [17] and variable-step boundary value methods based on reverse Adams method of order $p=6$ in [12] and Brugnano and Trigiante [14] using the extended trapezoidal rule of first kind $(ETRs)$ of order $p=6$, extended trapezoidal rule of second kind (ETR_2s) of order $p=6$ and top order methods $(TOMs)$ of order $p=6$. The rate is the numerical order of convergence, out in bracket. In all, the rate is in agreement with the order p of the respective methods in Tables 5 and 6.

Problem 2: Consider the non-linear system,

$$\begin{matrix} y_1' = -1002y_1 + 1000y_2^2, & y_1(0) = 1 \\ y_2' = y_1 - y_2(1 + y_2), & y_2(0) = 1 \end{matrix}, y(t) = \begin{pmatrix} e^{-2t} \\ e^{-t} \end{pmatrix}$$

in [42].

The SDGEBDFs3 is applied on problem 2 using a step length $h = 0.01$ on the interval of $0 < t \leq 10$. As in Table 7, the numerical results of the SDGEBDFs3 performs better for step sizes h=0.01 compared with the second derivative Adam's methods (SDAM) in [17] of order $p=6$, Block hybrid -second derivative methods (BHSDM) in [44] and Wu and Xia [42] with a smaller step length $h = 0.002$. Thus on Problem 2, the method (3.2) obtained better accuracy than the compared methods at lower dimension of the system of non-linear equation in (3.11).

Problem 3:A linear problem in [8, 16],

$$y' = \begin{pmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix};$$

The SDGEBDFs3 is applied to this problem with a fixed step size $h = 0.08$ and the maximium error $\left(\max \mid y_{1/h} - y(1) \mid\right)$ in the interval of $0 \leq t \leq 10$ is computed against the variable-step methods of 125 steps of iteration. From Table 8 that the SDGEBDFs3 performs better than the second derivative methods in [8] and Gear [43].

Problem 4: The problem is stiff initial value problem from chemistry;

$$y_1' = -0.03y_2 - 1000y_1y_2 - 2500y_1y_3$$
$$y_2' = -0.03y_2 - 1000y_1y_2$$
$$y_3' = -2500y_1y_3$$

with initial value $y_0 = (0, 1, 1)^T$. For t=2 the exact solution is $y(2) = \left(-0.361693316989 \times 10^{-5}, 0.981509948230, 1.018493388244\right)^T$. Table 9 contains numerical results of this problem and compared with methods from Hojjati *et al.* [10], Ismail [9], SDBDF [2] and MATLAB ODE15s [45].

Problem 5: Robertson's equation, [2]

$$y_1' = -0.04y_1 + 10^4y_2y_3, \quad y_2' = 0.04y_1 - 10^4y_2y_3 - 3 \times 10^7y_2^2,$$
$$y_3' = 3 \times 10^7 \quad y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0,$$

Table 10, contains the absolute error is given as the modulus of the ODE15s in MATLAB [45] minus the numerical solution of the SDGEBDFs3.

TABLE 5. numerical solution of problem 1, $t = 1$

Step	SDGEBDFs3 (rate)	SDAM [17] (rate)	Amodio6 [20] (rate)	Amodio8 [20] (rate)
20	2.00×10^{-5}	2.90×10^{-3}	5.70×10^{-2}	2.90×10^{-2}
	$(-)$	$(-)$	$(-)$	$(-)$
40	3.87×10^{-7}	7.30×10^{-5}	8.70×10^{-3}	6.80×10^{-3}
	(5.69)	(5.30)	(2.70)	(2.1)
80	8.77×10^{-9}	1.80×10^{-6}	4.9×10^{-4}	7.80×10^{-5}
	(5.46)	(5.30)	(4.20)	(6.40)
160	1.82×10^{-10}	3.30×10^{-8}	1.20×10^{-5}	4.71×10^{-7}
	(5.59)	(5.80)	(5.40)	(7.40)
320	3.29×10^{-12}	5.10×10^{-10}	2.20×10^{-7}	2.32×10^{-9}
	(5.79)	(6.00)	(5.80)	(7.71)
640	5.48×10^{-14}	7.70×10^{-10}	2.20×10^{-7}	1.31×10^{-11}
	(5.90)	(6.00)	(5.90)	(7.50)

6. CONCLUSION

This paper has presented SDGEBDFs for $k = 1(1)16$ based on the extended SDBDF as a SDBVM in (3.2) . In Tables 3 and 4, we reported the coefficients of the method in (3.2) for $k = 1(1)5$ and are found to be $O_{k,k-1}$–stable and $A_{k,k-1}$–stable. The proposed method

TABLE 6. numerical solution of problem 1 (continuation)

h	SDGEBDFs3 (rate)	ETRs [14] (rate)	ETR2s [14] (rate)	TOM [14] (rate)
2e-2	3.22×10^{-7} $(-)$	3.77×10^{-3} $(-)$	3.51×10^{-3} $(-)$	1.55×10^{-3} $(-)$
1e-2	3.79×10^{-9} (6.40)	1.00×10^{-4} (5.23)	8.62×10^{-5} (5.35)	9.77×10^{-6} (7.31)
5e-3	5.39×10^{-11} (6.14)	1.09×10^{-6} (6.53)	7.23×10^{-7} (6.90)	1.20×10^{-7} (6.35)
2.5e-3	8.89×10^{-13} (5.92)	1.79×10^{-8} (5.93)	8.86×10^{-9} (6.39)	1.85×10^{-9} (6.01)

TABLE 7. numerical solution of problem 2

Method	order p	h	s	y_1 $(\max \mid y_i - y_{t(i)} \mid)$	y_2 $(\max \mid y_i - y_{t(i)} \mid)$
SDGEBDFs3	6	0.01	20	1.47×10^{-22}	2.03×10^{-18}
SDGEBDFs3	6	0.01	120	3.70×10^{-23}	8.06×10^{-19}
SDAM [17]	6	0.008	125	1.63×10^{-14}	0.00
Wu and Xia[42]	7	0.002	500	2.56×10^{-07}	8.02×10^{-8}
BHSDM [44]	6	0.01	1000	7.09×10^{-22}	7.82×10^{-18}

TABLE 8. numerical solution of problem 3

Method	h	s	$Erry_1$	$Erry_2$	$Erry_3$	$Erry_4$
Enright[8]	0.08	125	0.44×10^{-6}	0.00	0.00	0.00
Gear[43]	0.08	422	1.06×10^{-6}	0.00	0.00	0.00
SDGEBDFs3	0.08	125	0.83×10^{-15}	0.00	0.00	0.00
SBDF[2]	0.001		1.35×10^{-6}	1.94×10^{-25}	4.20×10^{-45}	6.06×10^{-2}
SDLMM[9]	0.001		9.52×10^{-7}	1.5×10^{-25}	4.20×10^{-45}	0.00
SDGEBDFs3	0.001	25	1.99×10^{-16}	1.99×10^{-33}	0.00	0.00

(3.2) is stable at infinity for all k unlike that of SDEBDF of Cash [1] which stability is limited to $k \leq 9$. The SDGEBDFs of order p =6, $k = 3$ in (3.2) has been implemented on some standard problems with results presented in Tables 5, 6, 7, 8,9 and 10. The error constant (EC) of the proposed methods is smaller then the method of Enright [8], SDBDF [2], Ismail [9] and

TABLE 9. The error results of problem 4 at time $t = 2.0$

y_i	Error in SDGEBDFs3	Error in [10]	Error in [9]	Error in [2]	Error in ODE15s
y_1	0.95×10^{-19}	0.14×10^{-18}	0.82×10^{-10}	0.30×10^{-8}	0.28×10^{-12}
y_2	0.64×10^{-14}	0.23×10^{-13}	0.61×10^{-5}	0.18×10^{-5}	0.16×10^{-5}
y_3	0.86×10^{-13}	0.19×10^{-12}	0.57×10^{-5}	0.75×10^{-5}	0.54×10^{-5}

TABLE 10. Errors in problem 5 using $Erry_i =\mid y_i\,(3.12) - ODE15s(y_i) \mid$ $, i = 1(1)3, h = 0.0001$

t	$Erry_1$	$Erry_2$	$Erry_3$
1	1.34×10^{-7}	3.09×10^{-11}	1.35×10^{-7}
5	1.23×10^{-6}	5.50×10^{-10}	1.23×10^{-6}
10	3.23×10^{-5}	5.64×10^{-9}	3.23×10^{-5}

method of Hojjati etal [10]. Finally, the proposed method have the advantage of order p and stability as SDBVM in general than the compared methods.

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