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High Order Multi-block Boundary-value Integration Methods for Stiff ODEs

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Abstract

In this paper, we present a new family of multi-block boundary value integration methods based on the Enright second derivative type-methods for differential equations. We rigorously show that this class of multi-block methods are generally A_{k_1,k_2}-stable for all block number by verifying through employing the Wiener-Hopf factorization of a matrix polynomial to determine the root distribution of the stability polynomial. Further more, the correct implementation procedure is as well determine by Wiener-Hopf factorization. Some numerical results are presented and a comparison is made with some existing methods. The new methods which output multi-block of solutions of the ordinary differential equations on application, and are unlike the conventional linear multistep methods which output a solution at a point or the conventional boundary value methods and multi-block methods which output a block of solutions per step. The second derivative multi-block boundary value integration methods are a new approach at obtaining very large scale integration methods for the numerical solution of differential equations.

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1 Introduction

Recently, the notion of obtaining multi-block of solution values at each step of application rather than the block of solution values per step, or a single solution per step is recently receiving great attention. The first author to introduce such method is in [1], which take advantage of parallelism over the implementation of the conventional linear multistep methods. An extension of [1] can be found in [2]. Although, the introduction of block methods for non-stiff initial value problems is in [3, 4]. The [5] considered parallel block method for initial value problems. The use of parallel predictor-corrector was considered in [6]. Other authors on block methods are in [7–12]. In accordance with [13], the conventional linear multistep method (LMMs),

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}, \quad \alpha_k = 1, \quad n = 0, 1, \cdots, \tag{1.1}$$

has order and stability limitation for the numerical solution of the stiff initial value problems (IVPs)

$$\begin{aligned} y'(x) = f(y(x)), \quad x \in (x_0, X), \quad y(x_0) = y_0; \\ f : R \times R^m \to R^m; \quad y, y_0 \in R^m; \quad x_0, x \in R, \end{aligned} \tag{1.2}$$

in ordinary differential equations (ODEs) see [14–17]. This limitation gives room for new search for stiff solvers in LMM. However, the introduction of second derivative function to overcome this limitation was considered in [18, 19]. In [20], the second derivative linear multistep method (SDLMM) is,

$$y_{n+k} - y_{n+k} = h \sum_{j=0}^{k} \beta_j f_{n+j} + h^2 \gamma_k f'_{n+k}, \quad n = 0, 1, \cdots, \tag{1.3}$$

with $\{y_0, y_1, \cdots, y_{k-1}\}$ initial condition values. The first characteristics polynomial $\rho(r) = r^k(r - 1)$ is choosen for zero-stability and the third characteristics polynomial $\omega(r) = \gamma_k r^k$ is choosen for stability at infinity. The method in (1.3) is of order $p = k+1$ and is $A-$stable for $k = 1, 2$ and $A(\alpha)-$ stable for $k = 3(1)7$, with instability setting in when $k \geq 8$. Regardless the improved order, the second derivative LMMs are limited with A-stability condition with respect to their step number k. A new approach to circumvent the order and stability barrier in LMM for all step number k can be found in [21–31], where discretization of (1.2) is done by a boundary value method (BVM). This is a linear multistep method coupled with boundary value conditions (instead of initial value conditions). The next is a new result required to determine the formulation and the implementation of the proposed methods.

1.1 The Wiener-Hopf factorization and its application

In this subsection, we aim at factoring a matrix polynomial into two products of matrices, where the determinant of the first matrix contains all its roots in a unit circle and the second contains its roots outside the unit circle [32–34]. The Wiener-Hopf factorization can be defined for a matrix-valued function

$$C(R) = \sum_{i=-\infty}^{\infty} C_i R^i; \quad C_i \in C^{m\times m} \tag{1.4}$$

in the Wiener class W_m formed by all the functions $C(R)$ such that

$$\sum_{i=-\infty}^{\infty} \mid C_i \mid < \infty \tag{1.5}$$

$\mid F \mid = (\mid f_{i,j} \mid), \quad F = (a_{i,j})$ for $C(R) \in W_m$, the Wiener-Hopf factorization exist in the form

$$\begin{gathered} C(R) = F(R)diag(R^{k_1}, \cdots, R^{k_m})U(R^{-1}); \\ F(R) = \sum_{i=0}^{\infty} F_i R^i, \quad U(R) = \sum_{i=0}^{\infty} U_i R^i, \\ det(C(R)) \neq 0 \quad for \quad \mid R \mid = 1 \end{gathered}$$

Here $F(R)$, $U(R) \in W_m$ and $\det(F(r))$, $\det\,(U(r))$ are non-zero in the open unit disk. If the partial indices $k_i \in Z$ are zeros, the canonical factorization take the form

$$C(R) = F(R)U(R^{-1}). \tag{1.6}$$

Its matrix representation provides a block UL factorization of the infinite block Toeplitz matrix $TM(C_{j-i})$.

$$\begin{pmatrix} C_0 & C_1 & \cdots & \cdots \\ C_{-1} & C_0 & C_1 & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} F_0 & F_1 & \cdots & \cdots \\ \mathbf{0} & F_0 & F_1 & \cdots \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} U_0 & \mathbf{0} & \cdots & \cdots \\ U_{-1} & U_0 & \mathbf{0} & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tag{1.7}$$

Moreover, the condition $\det(F(r))$, $\det(U(r)) \neq 0$ for $\mid r \mid \leq 1$ provided the existence of $F(R)^{-1}$, $U(R)^{-1}$ in W_m, imply that the two infinite matrices have a block Toeplitz inverse which has bounded infinity norm. If the condition $\det(F(r))$, $\det(U(r)) \neq 0$, $\mid R \mid < 1$, for instance, there may exist $\hat{R}$ with $\mid \hat{R} \mid = 1$ such that $\det(F(\hat{r})) = 0$ then, the canonical factorization is said to be weak canonical factorization. In this case $F(R)$ or $U(R)$ may be not invertible in W_m e.g $F(R) = (1 - R)I$ has inverse $F(R)^{-1} = \sum_{i=0}^{\infty} IR^i$ which does not belong to W_m, see [34]. An application of the Wiener-Hopf factorization to obtain a second derivative multi-block boundary value method is illustrated in what follows. Consider the stability matrix polynomial

$$\widehat{\rho}(R) = A_1 R + A_0 - z(B_0 + B_1 R + B_2 R^2) - z^2 D_1 R; \quad z = \lambda h, \tag{1.8}$$

associated with a SDMB$_2$VMs in section 3 (ahead). The matrix coefficients are given as

$$A_1 = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}; \quad B_0 = \begin{pmatrix} -\frac{353}{120960} & \frac{1219}{4480} \\ -\frac{31}{120960} & \frac{29}{4480} \end{pmatrix}; \quad B_1 = \begin{pmatrix} \frac{1081}{2520} & \frac{2123}{7560} \\ \frac{3733}{7560} & \frac{3733}{7560} \end{pmatrix};$$
$$A_0 = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}; \quad B_2 = \begin{pmatrix} \frac{99}{4480} & -\frac{43}{40320} \\ \frac{29}{4480} & -\frac{31}{120960} \end{pmatrix}; \quad D_1 = \begin{pmatrix} -\frac{277}{672} & -\frac{289}{2016} \\ \frac{191}{2016} & -\frac{191}{2016} \end{pmatrix};$$

which correspond to a SDMB$_2$VMs that is $A_{1,1}$-stable. Here the case of $z = -6$ in (1.8) gives rise to the characteristics matrix polynomial $\widehat{\rho}_2(R) = F(R)U(R)$, which

$$\left(\begin{array}{c} A_0 - zB_0 \\ \hline A_1 - zB_1 - z^2 D_1 \\ A_2 - zB_2 \end{array}\right) = \left(\begin{array}{cc} \frac{19807}{20160} & \frac{3657}{2240} \\ -\frac{20191}{20160} & \frac{2327}{2240} \\ \hline \frac{14627}{840} & \frac{19771}{2520} \\ -\frac{1129}{2520} & \frac{1079}{320} \\ \frac{297}{2240} & -\frac{43}{6720} \\ \frac{87}{2240} & -\frac{31}{20160} \end{array}\right) = \left(\begin{array}{cccc} f_{01} & f_{02} & 0 & 0 \\ f_{03} & f_{04} & 0 & 0 \\ \hline 1 & 0 & f_{01} & f_{02} \\ 0 & 1 & f_{03} & f_{04} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{cc} u_{01} & u_{02} \\ u_{03} & u_{04} \\ u_{11} & u_{12} \\ u_{13} & u_{14} \end{array}\right). \tag{1.9}$$

Using Netwon-Raphson approach as in [32] to resolve this non-linear equation in (1.9), the Mathematica 11.1 version gives eleven options. However, we have chosen this

$$\begin{gathered} f_{01} = -7431.2, \quad f_{02} = 25816.3, \quad f_{03} = -2919.69, \quad f_{04} = 9955.48, \\ u_{01} = 0.02556, \quad u_{02} = -0.007578, \quad u_{03} = 0.007395, \quad u_{04} = -0.002118, \\ u_{11} = 0.132589, \quad u_{12} = -0.00639881, \quad u_{13} = 0.0388393, \quad u_{14} = -0.0015377. \end{gathered} \tag{1.10}$$

solution amongst the options. This leads to right hand canonical factorization amongst other options.

$$F(R) = \begin{pmatrix} -7431.2 & 25816.3 \\ -2919.69 & 9955.48 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} R = F_0 + F_1 R \tag{1.11}$$

where the roots of the det $(F(r))$ gives two real outside the unit circle; $r_1 = -1708.01$ and $r_2 = -816.273$. From (1.10),

$$U(R) = \begin{pmatrix} 0.02556 & -0.007578 \\ 0.007395 & -0.002118 \end{pmatrix} + \begin{pmatrix} 0.132589 & -0.006398 \\ 0.038839 & -0.001537 \end{pmatrix} R = U_{-1} + U_0 R \tag{1.12}$$

Similarly, the roots of the det $(U(r))$ gives two real roots inside the unit circle; $r_3 = -0.36484$ and $r_4 = -0.116696$. The existence of the Wiener-Hopf factorization above gives the band structured block Toeplitz matrix

$$A = \begin{pmatrix} A_1 & \mathbf{O} & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ A_0 & A_1 & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & A_0 & A_1 & \mathbf{O} & \cdots & \mathbf{O} \\ & & & \ddots & & \\ \mathbf{O} & \cdots & \mathbf{O} & A_0 & A_1 & \mathbf{O} \\ \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} & A_0 & A_1 \end{pmatrix};$$

$$B = \begin{pmatrix} B_1 & B_2 & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ B_0 & B_1 & B_2 & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & B_0 & B_1 & B_2 & \cdots & \mathbf{O} \\ & & & & \ddots & \\ \mathbf{O} & \cdots & \mathbf{O} & B_0 & B_1 & B_2 \\ \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & B_0 & B_1 \end{pmatrix}; \tag{1.13}$$

$$D = \begin{pmatrix} D_1 & \mathbf{O} & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & D_1 & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & D_1 & \mathbf{O} & \cdots & \mathbf{O} \\ & & & & \ddots & \\ \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} & D_1 & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} & D_1 \end{pmatrix},$$

The result is the 2-block, 2-point SDBVM

$$AY - hBF - h^2DF' = \begin{pmatrix} -A_0Y_n + hB_0F_n, & \mathbf{O}, & \cdots, & \mathbf{O}, & hB_2F_{n+N} \end{pmatrix}^T, \tag{1.14}$$

where Y, F, F' are defined in (3.15).

In this paper, a family of multi-block boundary value method based on the Enright type-method through [1] with the purpose of improving the order and stability properties will be introduced. The article is organized as follows: In Section 2, a brief introduction of second derivative multi-block methods on initial and boundary method is presented along their stability criteria. In Section 3, derivation of multi-block generalized second derivative linear multistep methods based on the methods of [20] is presented. Section 4, contain the application of second derivative MB_2VMs on Amenable differential algebraic equations, while Section 5, is on the implementation of the proposed methods and the conclusion follows in Section 6.

2 Second Derivative Multi-block Boundary Value Integration Methods

The extension of linear multi-block methods of [1] to second derivative is of the form,

$$\sum_{j=0}^{k} A_j Y_{n+j} = h \sum_{j=0}^{k} B_j F_{n+j} + h^2 \sum_{j=0}^{k} D_j F'_{n+j}; \quad n = 0, 1, \cdots : \quad k \geq 1. \tag{2.1}$$

obtained from [2] when $q = 2$, $\mu = s$, where

$$\begin{aligned} A_j &= \left[a_{i,l}^{(j)}\right]_{i,l=1(1)s}, \quad B_j = \left[b_{i,l}^{(j)}\right]_{i,l=1(1)s}, \\ Y_{n+j} &= \left(y_{n+s\cdot j}, y_{n+s\cdot j+1}, \cdots, y_{n+s\cdot j+s-1}\right)^T, \quad j = 0(1)k \\ F_{n+j} &= \left(f_{n+s\cdot j}, f_{n+s\cdot j+1}, \cdots, f_{n+s\cdot j+s-1}\right)^T \\ F'_{n+j} &= \left(f'_{n+s\cdot j}, f'_{n+s\cdot j+1}, \cdots, f'_{n+s\cdot j+s-1}\right)^T. \end{aligned} \tag{2.2}$$

The $\{Y_{n+j}\}_{j=0(1)k}$ are the multi-block of non-overlapping solution values, and $\{F_{n+j}\}_{j=0(1)k}$ and $\left\{F'_{n+j}\right\}_{j=0(1)k}$ denote the corresponding multi-block of non-overlapping function and derivative function values of (2.1) respectively. The formula (2.1) is a k-block, s-point block second derivative formula. Here, the block shift operator E is defined as $E^j Y_n = Y_{n+j}$. Here the first, second and third characteristics matrix polynomial of (2.1) as

$$\widehat{\rho}(R) = \sum_{j=0}^{k} A_j R^j, \qquad \widehat{\sigma}(R) = \sum_{j=0}^{k} B_j R^j, \qquad \widehat{\varsigma}(R) = \sum_{j=0}^{k} D_j R^j \tag{2.3}$$

respectively. The first, second and third characteristic stability polynomial of (2.1) are

$$\rho(r) = det\left(\widehat{\rho}(r)\right) = det\left(\sum_{j=0}^{k} A_j r^j\right), \quad \sigma(r) = det\left(\sum_{j=0}^{k} B_j r^j\right), \quad \varsigma(r) = det\left(\sum_{j=0}^{k} D_j r^j\right). \tag{2.4}$$

The stability matrix polynomial of (2.1) on application on the scalar test equation

$$y' = \lambda y; \quad Re(\lambda) < 0 \tag{2.5}$$

is

$$\widehat{\prod}(R, z) = \widehat{\rho}(R) - z\widehat{\sigma}(R) - z^2\widehat{\varsigma}(R); \quad z = \lambda h \tag{2.6}$$

The corresponding stability polynomial associated with (2.1) is thus,

$$\begin{aligned} \prod(r, z) = det\left(\widehat{\prod}(r, z)\right) = det\left(\widehat{\rho}(r) - z\widehat{\sigma}(r) - z^2\widehat{\varsigma}(r)\right); \\ r = e^{j\theta}, \quad 0 < \theta \leq 2\pi, \quad z = \lambda h, \quad Re(z) < 0 \end{aligned}. \tag{2.7}$$

Due to the A-stability limitation of multi-block in [1] and Daniel-Moore conjecture in [16], we consider the approach in [23, 26] on second derivative of [1] with the condition in subsection 1 holds. The second derivative multi-block boundary value methods ($SDMB_2VMs$) to be considered are a large scale of integration methods for numerical approximation of differential equations based on the conventional initial value multi-block methods in [1, 2]. However, The multi-block boundary value methods (MB_2VMs) is first introduced in [35]. Herein, the $SDMB_2VMs$ is described by,

$$\sum_{j=-k_1}^{k_2} A_{j+k_1} Y_{n+j} = h \sum_{j=-k_1}^{k_2} B_{j+k_1} F_{n+j} + h^2 \sum_{j=-k_1}^{k_2} D_{j+k_1} F'_{n+j}; \qquad \begin{matrix} n = 0(1)(N-k) \\ k > 1, \quad k = k_1 + k_2 \end{matrix}$$

$$\underbrace{Y_0, \cdots, Y_{k_1-1}}_{\text{(a)}} \qquad \underbrace{Y_{k_1}, \cdots, Y_{N-k_2}}_{\text{multi-block of solution values to be generated by the SDMB}_2\text{VMs}} \qquad \underbrace{Y_{N-k_2+1}, \cdots, Y_N}_{\text{(b)}} \tag{2.8}$$

as the main block formula while the initial multi-block solution values (a) and final multi-block solution values (b) in (2.8) are to be provided or replaced by multi-block second derivative multistep formulas. The $SDMB_2VMs$ in (2.8) is a k-block, s-point SDBVM. The coefficients $\{A_j, B_j, D_j\}$ are determined by imposing a $O\left(h^{4s\cdot k+1}\right)$ truncation error. Here $q_1 = s \cdot k_1$ is the number of roots lying inside the unit circle and $q_2 = s \cdot k_2$ is the number of roots lying outside the unit circle of the stability polynomial in (2.7) of the main methods in (2.8). Implementing (2.8) as a SDMB$_2$VMs, we shall have the discrete problem generated by a SDMB$_2$VMs (2.8) with (k_1, k_2)-block boundary conditions is written in the compact form

$$AY - hBF - h^2DF' = -\begin{pmatrix} \sum_{j=0}^{k_1-1}\left(A_jY_{n+j} - hB_jF_{n+j} - h^2D_jF'_{n+j}\right) \\ \vdots \\ A_0Y_{n+k_1-1} - hB_0F_{n+k_1-1} - h^2D_0F'_{n+k_1-1} \\ \mathbf{O} \\ \vdots \\ \mathbf{O} \\ A_kY_{n+N-k_2+1} - hB_kF_{n+N-k_2+1} - h^2D_kF'_{n+N-k_2+1} \\ \vdots \\ \sum_{j=1}^{k_2} A_{k_1+j}Y_{n+N-k_2+j} - hB_{k_1+j}F_{n+N-k_2+j} - h^2D_{k_1+j}F'_{n+N-k_2+j} \end{pmatrix} \tag{2.9}$$

where

$$\begin{aligned} Y = \left(Y_{n+k_1}, \cdots, Y_{n+N-k_2}\right)^T, \quad F = \left(F_{n+k_1}, \cdots, F_{n+N-k_2}\right)^T \\ F' = \left(F'_{n+k_1}, \cdots, F'_{n+N-k_2}\right)^T \end{aligned} \tag{2.10}$$

as the multi-block solution, function and derivative vectors of (2.9) respectively. The A, B and D are the multi-block Toeplitz matrices obtained from the main formula (2.8) without the initial multi-block second derivative formulas and final multi-block second derivative formulas. The arising SDMB$_2$VMs in (2.8) is thus A_{k_1,k_2}-stable. The multi-block Toeplitz matrix A is of the form

$$A = \begin{pmatrix} A_{k_1} & A_{k_1+1} & \cdots & A_k & \mathbf{O} & \mathbf{O} & \cdots & \cdots & \mathbf{O} \\ \vdots & \ddots & & & & & & & \vdots \\ A_1 & & \ddots & & & & & & \vdots \\ A_0 & & & & & & & & \vdots \\ \mathbf{O} & \ddots & & & \ddots & & & & \vdots \\ \mathbf{O} & & \ddots & & & \ddots & & & A_k \\ \vdots & & & \ddots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & & & \ddots & A_{k_1+1} \\ \mathbf{O} & \cdots & \cdots & \mathbf{O} & \mathbf{O} & A_0 & A_1 & \cdots & A_{k_1} \end{pmatrix}_{(N-k)s\times(N-k)s} ; k_1 + k_2 = k \tag{2.11}$$

where B and D is of a similar form, but with the $B_j's$ and $D_j's$ respectively, instead of the $A_j's$. The coefficient block matrices are Toeplitz-block matrices having lower band k_1 (equal to the number of block initial conditions) and upper band k_2 (equal to the number of block final conditions). The continuous problem in (1.2) gives only the initial value y_0, whereas the remaining $k-1$ blocks additional solution values in (2.8) are not known. However, the k_1 extra initial blocks $Y_0, \cdots, Y_{k_1-1}$ $(n=0)$, of solution values in (2.9) can be provided by the initial block second derivative formulas,

$$\sum_{j=0}^{k} A_j^{(i)} Y_j = h \sum_{j=0}^{k} B_j^{(i)} F_j + h^2 \sum_{j=0}^{k} D_j^{(i)} F_j'; \quad i = 0(1)k_1 - 1, \tag{2.12}$$

and the k_2 extra final blocks $Y_N, \cdots, Y_{N+k_2-1}$ of solution values are provided by the final block second derivative formulas,

$$\sum_{j=0}^{k} A_{N-k+j}^{(i)} Y_{N-k+j} = h \sum_{j=0}^{k} B_{N-k+j}^{(i)} F_{N-k+j} + h^2 \sum_{j=0}^{k} D_{N-k+j}^{(i)} F_{N-k+j}'; \quad i = (N-k_2+1)(1)N. \tag{2.13}$$

The composite matrix scheme, (2.8), (2.12) and (2.13) which is a SDMB$_2$VMs is of uniform order p. Thus the composition is written in higher dimensional space as,

$$A_N Y - h B_N F - h^2 D_N F' = \mathbf{O}, \quad \mathbf{O} = (\mathbf{O}, \cdots, \mathbf{O})^T \tag{2.14}$$

Here the multi-block of solutions and functions are given as

$$\begin{aligned} Y &= (Y_n, \cdots, Y_{n+k_1-1}, Y_{n+k}, \cdots, Y_{n+N-k_2}, Y_{n+N-k_2+1}, \cdots, Y_{n+N})^T, \\ F &= (F_n, \cdots, F_{n+k_1-1}, F_{n+k}, \cdots, F_{n+N-k_2}, F_{n+N-k_2+1}, \cdots, F_{n+N})^T, \\ F' &= \left(F_n', \cdots, F_{n+k_1-1}', F_{n+k}', \cdots, F_{n+N-k_2}', F_{n+N-k_2+1}', \cdots, F_{n+N}'\right)^T \end{aligned} \tag{2.15}$$

and $A_N = \left[a \mid \bar{A}_N\right] \in R^{Ns\times(N+1)s}$ is

$$A_N = \left(\begin{array}{c|cccccc} A_0^{(1)} & A_1^{(1)} & \cdots & A_k^{(1)} & & & \\ \vdots & \vdots & \ddots & \vdots & & & \\ A_0^{(k_1-1)} & A_1^{(k_1-1)} & \cdots & A_k^{(k_1-1)} & & & \\ A_0 & A_1 & \cdots & A_k & & & \\ & A_0 & A_1 & \cdots & A_k & & \\ & & \ddots & \ddots & \cdots & \ddots & \\ & & & A_0 & A_1 & \cdots & A_k \\ & & & A_0^{(N-k_2+1)} & A_1^{(N-k_2+1)} & \cdots & A_k^{(N-k_2+1)} \\ & & & \vdots & \vdots & \cdots & \vdots \\ & & & A_0^{(N)} & A_1^{(N)} & \cdots & A_k^{(N)} \end{array}\right), \tag{2.16}$$

and $B_N = \left[b \mid \bar{B}_N\right]$, $D_N = \left[d \mid \bar{D}_N\right] \in R^{Ns\times(N+1)s}$ is of similar form, but with $B_j's$ and $D_j's$ instead of $A_j's$. The matrix $A_N - hB_N - h^2D_N$, has a multi-block quasi-Toeplitz structure [36–38] as a result of the additional multi-block second derivative formulas from (2.12, 2.13). The (2.14) is equivalent to the one-block method

$$\bar{A}_N\bar{Y}_{n+1} + \bar{A}_0\bar{Y}_n = h\left(\bar{B}_N\bar{F}_{n+1} + \bar{B}_0\bar{F}_n\right) + h^2\left(\bar{D}_N\bar{F}'_{n+1} + \bar{D}_0\bar{F}'_n\right) \tag{2.17}$$

in higher dimensional block with multi-block of solution output. Here the multi-block of solution, function and derivative function values are given as

$$\begin{aligned} \bar{Y}_{n+1} &= \left(Y_{n+1}, \cdots, Y_{n+k_1-1}, Y_{n+k}, \cdots, Y_{n+N-k_2}, Y_{n+N-k_2+1}, \cdots, Y_{n+N}\right)^T, \\ \bar{F}_{n+1} &= \left(F_{n+1}, \cdots, F_{n+k_1-1}, F_{n+k}, \cdots, F_{n+N-k_2}, F_{n+N-k_2+1}, \cdots, F_{n+N}\right)^T \\ \bar{F}'_{n+1} &= \left(F'_{n+1}, \cdots, F'_{n+k_1-1}, F'_{n+k}, \cdots, F'_{n+N-k_2}, F'_{n+N-k_2+1}, \cdots, F'_{n+N}\right)^T \end{aligned} \tag{2.18}$$

$$\bar{A}_0 = [\bar{a} \mid a] = \left(\begin{array}{c|c} & A_0^{(1)} \\ & \vdots \\ & A_0^{(k_1-1)} \\ & A_0 \\ \mathbf{O}_{(N-1)s\times Ns} & \mathbf{O} \\ & \vdots \\ & \mathbf{O} \end{array} \right); \bar{B}_0 = \left[\bar{b} \mid b\right] = \left(\begin{array}{c|c} & B_0^{(1)} \\ & \vdots \\ & B_0^{(k_1-1)} \\ & B_0 \\ \mathbf{O}_{(N-1)s\times Ns} & \mathbf{O} \\ & \vdots \\ & \mathbf{O} \end{array} \right) \tag{2.19}$$

$$\bar{D}_0 = \left[\bar{d} \mid d\right] = \left(\begin{array}{c|c} & D_0^{(1)} \\ & \vdots \\ & D_0^{(k_1-1)} \\ & D_0 \\ \mathbf{O}_{(N-1)s\times Ns} & \mathbf{O} \\ & \vdots \\ & \mathbf{O} \end{array} \right) \tag{2.20}$$

We define the following definitions.

Definition 2.1. The SDMB_2VMs (2.9) is *pre-consistent* if $\| (\bar{A}_N)^{-1}a \|_\infty = 1$ holds.

Definition 2.2. A matrix polynomial $\widehat{\rho}(R)$ of degree $k = k_1 + k_2$ in (2.3) is an S_{k_1,k_2}-*matrix polynomial*, if the roots $\{r_j\}_{j=1}^q$ of the polynomial $\rho(r)$ are such that

$$| r_1 |\leq \cdots \leq| r_{q_1} |< 1 <| r_{q_1+1} |\leq \cdots | r_q |, \quad q_1 + q_2 = q = s \cdot k. \tag{2.21}$$

Definition 2.3. A matrix polynomial $\widehat{\rho}(R)$ of degree $k = k_1 + k_2$ in (2.3) is an N_{k_1,k_2}-*matrix polynomial*, if the roots $\{r_j\}_{j=1}^q$ of the polynomial $\rho(r)$ in (2.4) are such that

$$| r_1 |\leq \cdots \leq| r_{q_1} |\leq 1 <| r_{q_1+1} |\leq \cdots | r_q |, \quad q_1 + q_2 = q = s \cdot k. \tag{2.22}$$

Definition 2.4. The SDMB_2VM (2.9) with (k_1, k_2)-block boundary conditions where $k = k_1 + k_2$ is ;

(a) O_{k_1,k_2}-*stable* if the corresponding first characteristics matrix polynomial $\widehat{\rho}(R)$ in (2.3) is a N_{k_1,k_2}- matrix polynomial with $q_1 = s \cdot k_1$ and $q_2 = s \cdot k_2$.

(b) (k_1, k_2)-*absolutely stable* for a given $z \in \mathbb{C}$, if the corresponding matrix polynomial $\widehat{\prod}(R, z)$ in (2.6) is a S_{k_1,k_2}- matrix polynomial.

(c) The region $D_{k_1,k_2} = \{z \in \mathbb{C} : \widehat{\prod}(R, z) \text{ in (2.6) is a } S_{k_1,k_2}\text{-matrix polynomial}\}$ is said to be *the region of* (k_1, k_2)-*absolute stability.*

(d) A_{k_1,k_2}-*stable* if $\bar{\mathbb{C}} \subseteq D_{k_1,k_2}$.

The A_{k_1,k_2}-stability define the stability of the SDMB_2VMs in terms of the block number k which is the degree of the stability matrix polynomial (2.6). It can as well be referred to as A_{k_1,k_2}-block stability.

Definition 2.5. A SDMB_2VMs in (2.17) is called a *minimum multi-block boundary value methods* if the dimension $N \cdot s$ is equal to the block number k. In fact from (2.16), we have

$$\widehat{A} \equiv [a|A] = \left(\begin{array}{c|ccc} A_0^{(1)} & A_1^{(1)} & \cdots & A_k^{(1)} \\ \vdots & \vdots & & \vdots \\ A_0^{(k)} & A_1^{(k)} & \cdots & A_k^{(k)} \end{array}\right), \quad \widehat{B} \equiv [b|B] = \left(\begin{array}{c|ccc} B_0^{(1)} & B_1^{(1)} & \cdots & B_k^{(1)} \\ \vdots & \vdots & & \vdots \\ B_0^{(k)} & B_1^{(k)} & \cdots & B_k^{(k)} \end{array}\right) \tag{2.23}$$

$$\widehat{D} \equiv [d|D] = \left(\begin{array}{c|ccc} D_0^{(1)} & D_1^{(1)} & \cdots & D_k^{(1)} \\ \vdots & \vdots & & \vdots \\ D_0^{(k)} & D_1^{(k)} & \cdots & D_k^{(k)} \end{array}\right) \tag{2.24}$$

Note in particular, the definition (2.5) shows that the maximum order of the k-block methods in (2.8) defining the minimum SDMB_2VMs in (2.17), see [12]. The next theorem shows the existence of the solution of SDMB_2VMs in (2.8).

Theorem 2.1. *Suppose that the matrix roots of the characteristics matrix polynomial*

$$\widehat{\rho}(R) = \sum_{j=0}^{k} A_j R^j \tag{2.25}$$

associated with

$$\sum_{j=0}^{k} A_j Y_{n+j} = 0; \quad n = 0, 1, \cdots; \qquad \underbrace{Y_0, Y_1, \cdots, Y_{k-1}, \quad Y_{N-k_1+1}, \cdots, Y_N}_{\text{initial and final multi-block of solution values to be provided}} \tag{2.26}$$

are such that,

$$\| L_{k_1-1} \|_\infty < \| L_{k_1} \|_\infty < \| L_{k_1+1} \|_\infty, \qquad \| L_{k_1} \|_\infty \leq 1. \tag{2.27}$$

Then the multi-block solution of the boundary value finite difference equation associated with (2.26) *having* k_1 *number of initial block conditions and* k_2 *number of final block conditions in*

$$\begin{aligned} Y_0 = C\eta^0 G, \quad Y_1 = C\eta^1 G, \cdots, \quad Y_{k_1-1} = C\eta^{k_1-1} G, \\ Y_{N-k_2+1} = C\eta^{N-k_2+1} G, \quad \cdots \quad, Y_N = C\eta^N G. \end{aligned} \tag{2.28}$$

has a solution for n *and* $N - n$ *sufficiently large. In fact, the multi-block solution of* (2.26) *subject to* (2.28) *behaves asymptotically as*

$$Y_n = R_{k_1}^n \left(\alpha + O\left(l_1^n\right) + O\left(l_1^{N-n}+\right) + O\left(l_3^{-N}\right)\right) + O\left(l_3^{N-n}\right); \quad n = 0, 1, \cdots, \tag{2.29}$$

where the vector α *depends on* $Y_0, Y_1, \cdots, Y_{k_1-1}$ $(n = 0)$ *and*

$$\left\{ \begin{aligned} l_1 = \| L_{k_1}^{-1} L_{k_1-1} \|_\infty < 1, \quad k_1 + k_2 = k \\ l_3 = min\left\{ | r_{s\cdot k_1+1} |, | r_{s\cdot k_1+2} |, \cdots, | r_{s\cdot k_1+s} | \right\} > 1, \\ l_2 = \| L_{k_1+1}^{-1} L_{k_1} \|_\infty < 1, \quad l_4 = \| L_{k_1-1} \|_\infty < 1, \\ L_{j+1} = diag\left(r_{s\cdot j+1}, r_{s\cdot j+2}, \cdots, r_{s\cdot j+s}\right), \quad j = 0(1)k-1 \\ \| L_{k_1} \|_\infty = \max\{| r_{s(k_1-1)+1} |, | r_{s(k_1-1)+2} |, \cdots, | r_{s\cdot k_1} |\} \leq 1; \\ | r_{s\cdot k_1} | = 1, \quad 1 < | r_{s\cdot k_1+r} |, \quad r = 1(1)s \end{aligned} \right. . \tag{2.30}$$

Proof. The proof is in [35], where $R_{k_1}^n$ is the generating matrix root (solvent). □

Theorem 2.2. *Given the stability polynomial* $\prod(r,z)$ *in* (2.7)*, we have* $\prod(r,z) = 0$ *which defines a map between the complex r-plane and the complex z plane,*

$$z(r) = det(\widehat{\rho}(r) - z\widehat{\sigma}(r) - z^2\widehat{\varsigma}(r)) \tag{2.31}$$

where $r \in \mathbf{C}$ *is a root of the stability polynomial* $\prod(r,z)$ *such that* $z = z(r)$.

The following holds.

The set

$$\tau = \left\{ z \in \mathbf{C} : z = z(e^{i\theta}), 0 \le \theta < 2\pi \right\} \tag{2.32}$$

Here, the set τ is the set associating to the roots on the boundary of the unit circle and is known as the boundary locus, see the similar case of linear multistep formula in section 4.7.1 in [23].

3 Multi-block Generalized Second Derivative LMF based on Method's of Enright.

Consider an initial multi-block generalized second derivative linear multistep method based on the Enright type-method (MBGEMs),

$$A_k Y_{n+k} + A_{k-1} Y_{n+k-1} = h \sum_{j=0}^{k} B_j F_{n+j} + h^2 D_{k,a} F'_{n+k}; \quad \begin{matrix} k \ge 1; \quad a = 1,2 \\ n = 0,1,\cdots, \end{matrix}$$

$$\underbrace{Y_0, Y_1, \cdots, Y_{k-1}}_{\text{(block solution values to be provided)}} \tag{3.1}$$

in order to get Y_k, Y_{k+1}, Y_{k+2}, $\cdots$; in a step by step fashion, with

$$A_k = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 1 & 0 & \ddots & 0 & 0 \\ 0 & -1 & 1 & \ddots & \vdots & 0 \\ 0 & 0 & -1 & \ddots & 0 & 0 \\ & \vdots & \vdots & \ddots & 1 & 0 \\ 0 & 0 & 0 & \ddots & -1 & 1 \end{pmatrix}_{s\times s}, \quad A_{k-1} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & \vdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ & \vdots & & \ddots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{s\times s}, \tag{3.2}$$

and

$$D_{k,a} = \begin{cases} D_{k,1}; & \texttt{diagonal matrix}, \quad a = 1 \\ D_{k,2}; & \texttt{dense matrix}, \quad a = 2 \end{cases} \tag{3.3}$$

Here, the coefficient matrices B_j, $D_{k,a}$ are strictly determined to have maximum order $p = s(k+2)$. The MBGEM in (3.1) of order $p = 3s$ is A-stable for fixed block number $k = 1$ and increasing block size $s = 2(1)5$, $D_{k,2}$ and $A(\alpha)$-stable for $s = 6$ and instability set in from $s \geq 7$. The method in (3.1) is also of order $p = 2(k+2)$ and is $A-$stable for $k = 1$, $D_{k,2}$ and $A(\alpha)-$ stable for $k = 2(1)7$, and become unstable at $k \geq 8$. To overcome the order and stability barrier in (3.1), we transform (3.1) to

$$A_u Y_{n+u} + A_{u-1} Y_{n+u-1} = h \sum_{j=0}^{k} B_j F_{n+j} + h^2 D_{u,a} F'_{n+u} \quad u \neq k, \quad k \geq 1; \quad n = 0, 1, \cdots,$$

$$\underbrace{Y_0, Y_2, \cdots, Y_{u-1}}_{\text{(a1)}} \quad \underbrace{Y_u, \cdots, Y_{N-k+u}}_{\text{solution values to be generated by the SDMB}_2\text{VM}} \quad \underbrace{Y_{N-k+u+1}, \cdots, Y_N}_{\text{(a2)}} \tag{3.4}$$

as the main formula in a second derivative multi-block boundary value method implementation. The coefficient matrices $A_u \equiv A_k$ and $A_{u-1} \equiv A_{k-1}$ in (3.2). The multi-block solution values $(a1)$ and $(a2)$ in (3.4) are to be provided or replaced by second derivative block linear multistep formulae. Considering (3.4) as a second derivative multi-block boundary value methods (SDMB$_2$VMs) with $u \neq k$, we gain the freedom of choosing the appropriate values of u that provide methods having the best stability properties for all block number $k \geq 1$. Here, u is define as

$$u = \begin{cases} \frac{k+1}{2}; & k \quad odd \\ \frac{k}{2}; & k \quad even \end{cases}; \quad k = 1, 2, 3, \cdots; \tag{3.5}$$

Here, the first characteristics polynomial $\rho(r)$ for a method in (3.4) is of degree sk with $s(k-u)$ number of roots at infinity, such that

$$\alpha_{sk} = \alpha_{sk-1} = \cdots = \alpha_{s(u+1)} = 0; \qquad u \geq 1.$$

Thus for $u = k$, the (3.4) is the conventional second derivative methods in (3.1). The $k+2$ matrix coefficients $\{B_j\}_{j=0}^{k}$ and D_u allow the construction of methods from (3.4) of maximal order $p = s(k+2)$. However, D_u can be choosen as diagonal matrix or full matrix. The proposed methods shall be referred to as multi-block generalized second derivative linear multistep methods of Enright (MBGSDLMME). The corresponding local truncation error operator for the MBGSDLMME is,

$$\begin{aligned} L\left[Y_n(x_n); h\right] &= A_u Y_{n+1}(x_n) + A_{u-1} Y_n(x_n) \\ &= h \sum_{j=0}^{k} B_j(\mu) F\left(Y_{n+j}(x_n)\right) - h^2 F'(Y_{n+v}(x_n)); \end{aligned} \tag{3.6}$$

where

$$\begin{aligned} Y_{n+j}(x_n) &= \left(y\left(x_{n+js}\right), y\left(x_{n+js+1}\right), y\left(x_{n+js+2}\right), \cdots, y\left(x_{n+js+s-1}\right)\right)^T \\ F^{(l-1)}\left(Y_{n+j}(x_n)\right) &= \Big(f^{(l-1)}\left(x_{n+js}, y\left(x_{n+js}\right)\right), f^{(l-1)}\left(x_{n+js+1}, y\left(x_{n+js+1}\right)\right), \\ & f^{(l-1)}\left(x_{n+js+2}, y\left(x_{n+js+2}\right)\right), \cdots, f^{(l-1)}\left(x_{n+js+s-1}, y\left(x_{n+js+s-1}\right)\right)\Big)^T \\ & \qquad l = 1, 2. \end{aligned}$$

The Taylor series about x_n in (3.6) gives

$$L\left[Y_n(x_n); h\right] = \sum_{j=0}^{\infty} \frac{C_j h^j}{j!} Y_{n+1}^{(j)}(x_n); \quad Y_n^{(j)}(x_n) = \underbrace{\left(y^{(j)}(x_n), y^{(j)}(x_n), \cdots, y^{(j)}(x_n)\right)^T}_{s}. \tag{3.7}$$

The next theorem holds for the MBGSDLMME.

Theorem 3.1.
Given $e = (1, \cdots, 1)^T$, the coefficients $\{C_x\}_{x=0}$ in (3.7) are given by

$$C_x = \begin{cases} e - A_u(s)e - A_{u-1}(s)e; & x = 0 \\ c - A_u(s)(c + sje) - A_{u-1}(s)(c + sje) - \sum_{j=0}^{k} B_j(s)e; & x = 1 \\ c^2 - A_u(s)(c + sje)^2 - A_{u-1}(s)(c + sje)^2 - 2\sum_{j=0}^{k} B_j(s)(c + sje) & \\ -D_v(s)e; & x = 2 \\ c^3 - A_u(s)(c + sje)^3 - A_{u-1}(s)(c + sje)^3 & \\ -x\sum_{j=0}^{k} B_j(s)(c + sje)^2 - (x-1)D_v(s)(c + sve); & x = 3 \\ \vdots & \\ c^x - A_u(s)(c + sje)^x - A_{u-1}(s)(c + sje)^x & \\ -x\sum_{j=0}^{k} B_j(s)(c + sje)^{x-1} - (x-1)D_v(s)(c + sve)^{x-2}; & x = 4, 5, \cdots \end{cases}, \tag{3.8}$$

where $c = (c_1, c_2, \cdots, c_s)^T$.

The vector powers are component-wise power. The MBGSDLMME in (3.4) is pre-consistent if $C_0 = 0$ and consistent if it is of order at least $p > 1$, where $C_0 = 0$ and $C_1 = 0$. See page 249 in [35]. The l.t.e is given as $\bar{C}_{p+1} = \frac{C_{p+1}}{(p+1)!}$

To determine the stability matrix polynomial of the method in (3.4), on application of Dahlquist test problem in (2.5) on (3.4), here $R^j Y_n = Y_{n+j}$, $R^u Y_n = Y_{n+u}$ and u is given in (3.5) to give,

$$\bar{\prod}(R, z) = A_u R^u + A_{u-1} R^{u-1} - z\sum_{j=0}^{k} B_j R^j - z^2 D_{u,a} R^u. \tag{3.9}$$

The stability polynomial associated with MBGSDLMME in (3.4)is given as

$$\begin{aligned} \prod(r, z) &= det\left(A_u r^u + A_{u-1} r^{u-1} - z\sum_{j=0}^{k} B_j r^j - z^2 D_{u,a} r^u\right) \\ &= \sum_{j=1}^{q_1} a_j r^j - z\sum_{j=0}^{q} b_j r^j - z^2 b_{2u} r^{2u}, \end{aligned} \tag{3.10}$$

and the methods from (3.4) are found to be $A_{u,k-u}$-stable and can be used with $(u, k-u)$-block boundary conditions. The first characteristics stability polynomial possesses a unique structure of the form,

$$\rho(r) = det\left(A_u r^u + A_{u-1} r^{u-1}\right) = r^{q_1 - 1}(r-1), \tag{3.11}$$

second characteristics stability polynomial is,

$$\sigma(r) = det\left(\sum_{j=0}^{k} B_j r^j\right) = \sum_{j=0}^{q} b_j r^j, \quad q = s \cdot k \tag{3.12}$$

and third characteristics polynomials associated with (3.4).

$$\gamma(r) = \det\left(D_{u,a} r^u\right) = b_{2u} r^{2u} \tag{3.13}$$

The stability region of the MBGSDLMME in (3.4) are the unbounded region of the exterior of the closed curves for all $k \geq 2$ as shown in the boundary loci in Fig. 2 and 3 for $k = 2(1)13$. One can see, the sigma set of the proposed methods in (3.4) grows as the block number k (even) increases. Therefore MBGSDLMME in (3.4) are $A_{u,k-u}-$stable since, $\mathbb{C}^-$ is contained in the $(u, k-u)-$ absolutely stability region of (3.4). In fact, when D_u is strictly diagonal matrix or full matrix, the method in (3.4) is $A_{u,k-u}-$stable for fixed s, along with increasing block number k see, Fig. 1. However, for a fixed block number k and increasing blocksize s, the (3.4) is found to be $A_{u,k-u}-$stable when D_u is strictly diagonal and $A(\alpha)_{u,k-u}$-stable when D_U contains dense matrix. By introducing the block Toeplitz matrices (BT-matrices) $s\,(N-k) \times s\,(N-k)$

$$A = \begin{pmatrix} A_u & \mathbf{O} & \cdots & \mathbf{O} & & & \\ \vdots & \ddots & & & \ddots & & \\ A_0 & & \ddots & & & \ddots & \\ & \ddots & & \ddots & & & \mathbf{O} \\ & & \ddots & & \ddots & & \vdots \\ & & & \ddots & & \ddots & \mathbf{O} \\ & & & & A_0 & \cdots & A_u \end{pmatrix}$$

$$B = \begin{pmatrix} B_u & \cdots & B_k & & & \\ \vdots & \ddots & & \ddots & & \\ B_0 & & \ddots & & \ddots & \\ & \ddots & & \ddots & & B_k \\ & & & \ddots & \ddots & \vdots \\ & & & B_0 & \cdots & B_u \end{pmatrix}, \quad D = \begin{pmatrix} D_{u,a} & \mathbf{O} & & & & \\ \mathbf{O} & \ddots & \mathbf{O} & & & \\ & \ddots & \ddots & \ddots & & \\ \vdots & & \mathbf{O} & D_{u,a} & & \\ & & & \ddots & \ddots & \mathbf{O} \\ \mathbf{O} & & & & \mathbf{O} & D_{u,a} \end{pmatrix}$$

the discrete problem generated by a $k-$block SDMB$_2$VMs in (3.4) with $(u, k-u)-$ block boundary conditions can be written in the compact form

$$AY - hBF - h^2DF' = \begin{pmatrix} -A_{u-1}Y_{u-1} + h\sum_{j=0}^{u-1} B_jF_j \\ h\sum_{j=0}^{u-2} B_jF_j \\ \vdots \\ hB_0F_{u-1} \\ \mathbf{O} \\ \vdots \\ \mathbf{O} \\ hB_kF_{N-j+1} \\ \vdots \\ h\sum_{j=1}^{k-u} B_{u+j}F_N \end{pmatrix} \tag{3.14}$$

This is a set of nonlinear system of matrix equations, where

$$Y = (Y_u, \cdots, Y_{N-k+1})^T, \quad F = (F_u, \cdots, F_{N-k+1})^T, \quad F' = \left(F'_u, \cdots, F'_{N-k+1}\right)^T \tag{3.15}$$

are multi-block solution, multi-block function and multi-block derivative vectors. The A and B are the multi-block Toeplitz matrices obtained from the main formula (3.4) without the initial multi-block formulas and final multi-block formulas. The arising $\mathrm{SDMB_2VMs}$ in (3.4) is thus $A_{u,k-u}$-stable. The continuous problem (1.1) provides only the initial value y_0, whereas the $u-$ extra initial multi-block solution values $Y_0, Y_1, \cdots, Y_{u-1}$ of (3.4) can be given by the initial formulas

$$A_i^{(i)} Y_i + A_{i-1}^{(i)} Y_{i-1} = h \sum_{j=0}^{k} B_j^{(i)} F_j + h^2 D_u^{(i)} F_u'; \quad i = 1(1)u-1, \quad i = 0(1)u-1, \tag{3.16}$$

or

$$A_i^{(i)} Y_i + A_{i-1}^{(i)} Y_{i-1} = h \sum_{j=0}^{k} B_j^{(i)} F_j + h^2 D_{i,a}^{(i)} F_i'; \quad i = 1(1)u-1, \quad i = 0(1)u-1, \tag{3.17}$$

and $k-u$ extra final blocks $Y_{N-k+u+1}, \cdots, Y_N$, of multi-block solution values in (3.4) are given by the final block formula

$$A_i^{(i)} Y_{N+i} + A_{i-1}^{(i)} Y_{N+i-1} = h \sum_{j=0}^{k} B_j^{(i)} F_{N+j} + h^2 D_{u,a}^{(i)} F_{N+u}'; \quad i = 0(1)k-u-1. \tag{3.18}$$

or

$$A_i^{(i)} Y_{N+i} + A_{i-1}^{(i)} Y_{N+i-1} = h \sum_{j=0}^{k} B_j^{(i)} F_{N+j} + h^2 D_{i,a}^{(i)} F_{N+i}'; \quad i = 0(1)k-u-1. \tag{3.19}$$

Here $A_i^{(i)} \equiv A_u$ and $A_{i-1}^{(i)} \equiv A_{u-1}$. The composition in (3.4), (3.18) or (3.19), (3.18) or (3.19) is written in higher dimensional space of one block method (2.17) as

$$\bar{A}_N \bar{Y}_{n+1} + \bar{A}_0 \bar{Y}_n = h\left(\bar{B}_N \bar{F}_{n+1} + \bar{B}_0 \bar{F}_n\right) + h^2\left(\bar{D}_N \bar{F}_{n+1}' + \bar{D}_0 \bar{F}_n'\right) \tag{3.20}$$

where

$$\begin{aligned} \bar{Y}_{n+1} &= \left(Y_{n+1}, \cdots, Y_{n+k_1-1}, Y_{n+k}, \cdots, Y_{n+N-k_2}, Y_{n+N-k_2+1}, \cdots, Y_{n+N}\right)^T, \\ \bar{F}_{n+1} &= \left(F_{n+1}, \cdots, F_{n+k_1-1}, F_{n+k}, \cdots, F_{n+N-k_2}, F_{n+N-k_2+1}, \cdots, F_{n+N}\right)^T; \\ \bar{F}_{n+1}' &= \left(F_{n+1}', \cdots, F_{n+k_1-1}', F_{n+k}', \cdots, F_{n+N-k_2}', F_{n+N-k_2+1}', \cdots, F_{n+N'}\right)^T; \end{aligned} \tag{3.21}$$

The following condition holds for the convergence of the second derivative MB_2VMs in (3.20)

Lemma 3.1. *Suppose that the sequence* $\{e_{i+1}\}$ *satisfies the condition of the difference inequality*

$$e_{i+1} \leq (1+\alpha h_{i+1})\, e_i + m_{i+1}h_{i+1}; \quad i = 0, 1 \tag{3.22}$$

with the sequences $\{e_{i+1}\}$, $\{d_{i+1}\}$, $\{h_{i+1}\}$ *and* α *are positive integer, then*

$$e_{i+1} \leq \left(e_0 + \sum_{j=0}^{i} m_j h_j\right) exp\left(\alpha \sum_{r=0}^{i} h_r\right) \tag{3.23}$$

Theorem 3.2. *Suppose the effect of round-off error is insignificant and the* (1.2) *satisfies the following Lipschitz condition*

$$\| F(t,x) - F(t,\widehat{x}) \|_\infty \leq L \| x - \widehat{x} \|_\infty \tag{3.24}$$

for all $t \in [t_0, T]$ *and* x, $\widehat{x}$, $\in \mathbb{C}$. *The methods in* (3.4) *with* (k_1, k_2)*-block boundary condition is convergent of order* $p = s(k+2)$, *if is consistent and the definition 2.1 holds.*

Proof.
When the composite methods in (3.20) is used to approximate the solution of the ODEs in (1.2) with the initial multi-block solution values Y_0, Y_1, $\cdots$, Y_{k_1} and final multi-block solution values Y_{N-k_1+1}, $\cdots$, y_N. Then,

$$\begin{aligned}\widehat{Y}_{n+1} &= \left(Y_{n+1}, \cdots, Y_{n+k_1-1}, Y_{n+k}, \cdots, Y_{n+N-k_2}, Y_{n+N-k_2+1}, \cdots, Y_{n+N}\right)^T, \\ \widehat{F}_{n+1} &= \left(F_{n+1}, \cdots, F_{n+k_1-1}, F_{n+k}, \cdots, F_{n+N-k_2}, F_{n+N-k_2+1}, \cdots, F_{n+N}\right)^T \\ \widehat{F}'_{n+1} &= \left(F'_{n+1}, \cdots, F'_{n+k_1-1}, F'_{n+k}, \cdots, F'_{n+N-k_2}, F_{n+N-k_2+1}, \cdots, F'_{n+N}\right)^T;\end{aligned} \tag{3.25}$$

is the mult-block of solution and function values and the local truncation error is given as

$$\tau_{n+1}(h) = \bar{A}_N \widehat{Y}_{n+1} - h\bar{B}_N \widehat{F}_{n+1} - h^2 \bar{D}_N \widehat{F}'_{n+1} + \bar{A}_0 \widehat{Y}_n - h\bar{B}_0 \widehat{F}_n - h^2 \bar{D}_0 \widehat{F}'_n \tag{3.26}$$

subtracting (3.20) from (3.26) gives the global truncation error

$$\begin{aligned}\varepsilon_{n+1} = \widehat{Y}_{n+1} - \bar{Y}_{n+1} = (\bar{A}_N)^{-1}\tau_{n+1}(h) - (\bar{A}_N)^{-1}A_0(\widehat{Y}_n - \bar{Y}_n)\\ +h(\bar{A}_N)^{-1}\bar{B}_N(\widehat{F}_{n+1} - \bar{F}_{n+1}) + h(\bar{A}_N)^{-1}\bar{B}_0(\widehat{F}_n - \bar{F}_n)\\ +h^2(\bar{A}_N)^{-1}\bar{D}_N(\widehat{F}'_{n+1} - \bar{F}'_{n+1}) + h^2(\bar{A}_N)^{-1}\bar{D}_0(\widehat{F}'_n - \bar{F}'_n)\end{aligned} \tag{3.27}$$

for easy notation, let $\| (\bar{A}_N)^{-1}\bar{B}_N \|_\infty = \varphi$, $\| (\bar{A}_N)^{-1}\bar{B}_0 \|_\infty = \vartheta$, $\| (\bar{A}_N)^{-1}\bar{D}_N \|_\infty = \Psi$, $\| (\bar{A}_N)^{-1}\bar{D}_0 \|_\infty = \beta$, $e_0 = 0$, $e_{n+1} = \max_{0\le j\le n} \| \varepsilon_{n+1} \|_\infty$, $n = 0(1)W_t$.

The SDMB$_2$VMs in (3.20) is pre-consistent, see definition 2.1. Hence, the SDMB$_2$VMs in (3.20) is consistent for order $p = s(k+2)$. Then from (3.24), we have

$$\begin{aligned}\| \varepsilon_{n+1} \|_\infty = \| \varepsilon_n \|_\infty + L((h\varphi + h^2\Psi) \| \varepsilon_{n+1} \|_\infty + (h\vartheta + h^2\beta) \| \varepsilon_n \|)\\ + \| (\bar{A}_N)^{-1} \|_\infty \| \tau_{n+1}(h) \|_\infty\\ \le e_i + L((h\varphi + h^2\Psi)e_{i+1} + (h\vartheta + h^2\beta)e_i) + d \| (\bar{A}_N)^{-1} \|_\infty h^{2sk+1}\end{aligned} \tag{3.28}$$

here $d > 0$ is independent of h and $n = 0(1)W_t$. Suppose there exist a non-negative h_0, and $L(\varphi h_0 - \Psi h^2) < 1$ such that

$$e_{n+1} \le \left(\frac{1 - L(\varphi(h_0 - h) + \Psi(h_0^2 - h^2) - \vartheta h - \beta h^2)}{1 - L(\varphi h_0 + \Psi h_0^2)}\right) e_n + \frac{Jh^{s(k+2)+2}}{1 - L(\varphi h_0 + \Psi h_0^2)} \tag{3.29}$$

$0 < h \le h_0$, then from lemma (3.1), we have

$$e_{n+1} \le \frac{JT}{s(1 - L(\varphi h_0 + \Psi h_0^2))} \exp\left[\frac{L(\varphi + \vartheta + (\Psi + \beta)h_0)}{s(1 - L(\varphi h_0 + \Psi h_0^2))}\right] h^{s(k+2)+1} \tag{3.30}$$

where $J = d \| (\bar{A}_N)^{-1} \|_\infty$, $T = W_t\widehat{h} = W_tNs \cdot h$.

Hence,

$$\max_{1\le n\le W_t} \| \varepsilon_{n+1} \|_\infty \equiv O(h^{s(k+2)+1}) \tag{3.31}$$

□

For example, the matrix coefficients of eight order MBGSDLMME in (3.4) with $u = 1$, and $s = 2$, are given as

$$A_1 Y_{n+1} + A_0 Y_n = h(B_0 F_n + B_1 F_{n+1} + B_2 F_{n+2}) + h^2 D_{1,2} F'_{n+1} \tag{3.32}$$

$$A_0 = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}; A_1 = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}; B_1 = \begin{pmatrix} \frac{1081}{2520} & \frac{2123}{7560} \\ \frac{3733}{7560} & \frac{3733}{7560} \end{pmatrix}; \bar{C}_9 = \begin{pmatrix} \frac{1759)}{25401600} \\ \frac{289}{25401600} \end{pmatrix}$$
$$B_0 = \begin{pmatrix} -\frac{353}{120960} & \frac{1219}{4480} \\ -\frac{31}{120960} & \frac{29}{4480} \end{pmatrix}; B_2 = \begin{pmatrix} \frac{99}{4480} & -\frac{43}{40320} \\ \frac{29}{4480} & -\frac{31}{120960} \end{pmatrix}; D_1 = \begin{pmatrix} -\frac{277}{672} & -\frac{289}{2016} \\ \frac{191}{2016} & -\frac{191}{2016} \end{pmatrix}; \tag{3.33}$$

it is $A_{1,1}$-stable and can be used with one initial second derivative linear multistep formula (SDLMF)

$$y_1 - y_0 = h\left(\frac{10667 f_0}{40320} + \frac{7869 f_1}{4480} + \frac{11573 f_2}{7560} - \frac{5849 f_3}{2520} - \frac{1091 f_4}{4480} + \frac{1537 f_5}{120960}\right)$$
$$+h^2\left(\frac{4447 f'_1}{2016} + \frac{907 f'_2}{672}\right); \qquad C_9 = -\frac{26591}{25401600} \tag{3.34}$$

and one final additional block equation given by

$$A_0^{(N)} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}; A_1^{(N)} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix};$$
$$D_1^{(N)} = \begin{pmatrix} \frac{289}{2016} & \frac{277}{672} \\ -\frac{907}{672} & -\frac{4447}{2016} \end{pmatrix}; \bar{C}_9 = \begin{pmatrix} \frac{1759}{25401600} \\ -\frac{26591}{25401600} \end{pmatrix};$$
$$B_0^{(N)} = \begin{pmatrix} -\frac{43}{40320} & \frac{99}{4480} \\ \frac{1537}{120960} & -\frac{1091}{4480} \end{pmatrix}; B_1^{(N)} = \begin{pmatrix} \frac{2123}{7560} & \frac{1081}{2520} \\ -\frac{5849}{2520} & \frac{11573}{7560} \end{pmatrix}; \tag{3.35}$$
$$B_2^{(N)} = \begin{pmatrix} \frac{1219}{4480} & -\frac{353}{120960} \\ \frac{7869}{4480} & \frac{10667}{40320} \end{pmatrix};$$

Thus is conveniently written in one-block form in conformality with (3.20) as,

$$\bar{A}_N = \begin{pmatrix} A_1 & 0 & 0 & \cdots & \cdots & 0 & 0 \\ A_0 & A_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_0 & A_1 & 0 & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 & 0 \\ \vdots & & 0 & 0 & A_0 & A_1 & 0 \\ 0 & \cdots & 0 & 0 & 0 & A_1^{(N)} & A_2^{(N)} \end{pmatrix}$$
$$\bar{B}_N = \begin{pmatrix} B_1 & B_2 & 0 & \cdots & \cdots & 0 & 0 \\ B_0 & B_1 & B_2 & 0 & 0 & 0 & 0 \\ 0 & B_0 & B_1 & B_2 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots \\ \vdots & & 0 & 0 & B_0 & B_1 & B_2 \\ 0 & \cdots & 0 & 0 & B_0^{(N)} & B_1^{(N)} & B_2^{(N)} \end{pmatrix}, \quad (3.36)$$

$$\bar{D}_N = \begin{pmatrix} D_1 & \mathbf{O} & \mathbf{O} & \cdots & \cdots & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & D_1 & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & D_1 & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \ddots & \ddots & \ddots & \ddots & \ddots \\ \vdots & & \mathbf{O} & \mathbf{O} & \mathbf{O} & D_1 & \mathbf{O} \\ \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} & \mathbf{O} & D_1^{(N)} & \mathbf{O} \end{pmatrix} \quad (3.37)$$

$$\bar{A}_0 = \begin{pmatrix} & | & A_0 \\ 0_{(N-1)s\times Ns} & | & 0 \\ & | & 0 \\ & | & \vdots \\ & | & 0 \end{pmatrix}, \quad \bar{B}_0 = \begin{pmatrix} & | & B_0 \\ 0_{(N-1)s\times Ns} & | & 0 \\ & | & 0 \\ & | & \vdots \\ & | & 0 \end{pmatrix} \quad (3.38)$$

of dimension $Ns \times Ns$ respectively. An example of seventh order MBGSDLMME in (3.4) with $u = 1$, and $s = 2$, (here B_u contain diagonal matrix), is

$$A_1 Y_{n+1} + A_0 Y_n = h(B_0 F_n + B_1 F_{n+1} + B_2 F_{n+2}) + h^2 D_1 F'_{n+1} \quad (3.39)$$

$$A_0 = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}; A_1 = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}; B_1 = \begin{pmatrix} \frac{586}{945} & \frac{113}{1260} \\ \frac{463}{1260} & \frac{586}{945} \end{pmatrix}; \bar{C}_8 = \begin{pmatrix} -\frac{289}{846720} \\ \frac{191}{846720} \end{pmatrix}$$
$$B_0 = \begin{pmatrix} -\frac{107}{20160} & \frac{97}{315} \\ \frac{1}{756} & -\frac{347}{20160} \end{pmatrix}; B_2 = \begin{pmatrix} -\frac{277}{20160} & \frac{1}{756} \\ \frac{19}{630} & -\frac{37}{20160} \end{pmatrix}; D_1 = \begin{pmatrix} -\frac{271}{1008} & 0 \\ 0 & -\frac{191}{1008} \end{pmatrix}; \tag{3.40}$$

it is $A_{1,1}$-stable and can be used with one initial SDLMF

$$y_1 - y_0 = h\left(\frac{1139 f_0}{3780} + \frac{24293 f_1}{20160} - \frac{1777 f_2}{1260} + \frac{586 f_3}{945} + \frac{97 f_4}{315} - \frac{97 f_5}{4032}\right) - h^2 \frac{863 f_2'}{1008}; \qquad C_8 = \frac{4447}{846720} \tag{3.41}$$

and one final additional block equation given by

$$\begin{aligned} A_0^{(N)} &= \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}; A_1^{(N)} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}; \\ D_1^{(N)} &= \begin{pmatrix} -\frac{271}{1008} & 0 \\ 0 & -\frac{863}{1008} \end{pmatrix}; \bar{C}_8 = \begin{pmatrix} \frac{277}{282240} \\ -\frac{907}{282240} \end{pmatrix}; \\ B_0^{(N)} &= \begin{pmatrix} \frac{13}{2240} & -\frac{17}{210} \\ -\frac{37}{3780} & \frac{631}{6720} \end{pmatrix}; B_1^{(N)} = \begin{pmatrix} -\frac{254}{945} & \frac{137}{140} \\ -\frac{73}{140} & -\frac{254}{945} \end{pmatrix}; \\ B_2^{(N)} &= \begin{pmatrix} \frac{2521}{6720} & -\frac{37}{3780} \\ \frac{149}{105} & \frac{643}{2240} \end{pmatrix}; \end{aligned} \tag{3.42}$$

Example for $k = 2$, $s = 3$, one obtains the matrix coefficients of a tenth order MBGSDLMME in (3.4),

$$A_1 Y_{n+1} + A_0 Y_n = h(B_0 F_n + B_1 F_{n+1} + B_2 F_{n+2} + D_{2,1} G_{n+2} \tag{3.43}$$

where,

$$A_1 = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}; A_0 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \bar{C}_{11} = \begin{pmatrix} -\frac{69823}{2395008000} \\ \frac{263}{14968800} \\ -\frac{40321}{2395008000} \end{pmatrix};$$

$$B_1 = \begin{pmatrix} \frac{10908767}{18144000} & \frac{83423}{725760} & -\frac{25559}{907200} \\ \frac{640307}{1814400} & \frac{13903}{22680} & \frac{101741}{1814400} \\ -\frac{5557}{181440} & \frac{57517}{145152} & \frac{10965089}{18144000} \end{pmatrix}; B_2 = \begin{pmatrix} \frac{6151}{907200} & -\frac{4127}{3628800} & \frac{3391}{36288000} \\ -\frac{1241}{145152} & \frac{2129}{1814400} & -\frac{2497}{29030400} \\ \frac{6163}{226800} & -\frac{1069}{453600} & \frac{41}{290304} \end{pmatrix};$$

$$B_0 = \begin{pmatrix} \frac{2687}{7257600} & -\frac{3523}{453600} & \frac{71137}{226800} \\ -\frac{3391}{29030400} & \frac{643}{362880} & -\frac{58703}{3628800} \\ \frac{2497}{36288000} & -\frac{3233}{3628800} & \frac{5353}{907200} \end{pmatrix}; D_{1,1} = \begin{pmatrix} -\frac{441}{1600} & 0 & 0 \\ 0 & -\frac{2497}{11520} & 0 \\ 0 & 0 & -\frac{2497}{14400} \end{pmatrix};$$

Since it is $A_{1,1}$-stable, it can be implemented with one additional initial and final block equations from (3.16) and (3.18) respectively. Further example for $k = 2$, $s = 4$, one obtains the matrix coefficients of a twelfth order MBGSDLMME in (3.4),

$$A_1 Y_{n+1} + A_0 Y_n = h(B_0 F_n + B_1 F_{n+1} + B_2 F_{n+2} + D_{2,1} F'_{n+2} \tag{3.44}$$

where,

$$A_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}; A_0 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \bar{C}_{13} = \begin{pmatrix} -\frac{4010257}{1387736064000} \\ \frac{4522787}{2719962685440} \\ -\frac{92427157}{67999067136000} \\ \frac{106034111}{67999067136000} \end{pmatrix};$$

$$B_0 = \begin{pmatrix} -\frac{360233}{10762752000} & \frac{914845571}{1307674368000} & -\frac{79953451}{8717829120} & \frac{9199123573}{29059430400} \\ \frac{25797689}{2179457280000} & -\frac{61321669}{290594304000} & \frac{523498609}{261534873600} & -\frac{113923639}{7264857600} \\ -\frac{133787}{20432412000} & \frac{231294521}{2179457280000} & -\frac{16646251}{19372953600} & \frac{425662331}{87178291200} \\ \frac{5512813}{1017080064000} & -\frac{53896501}{653837184000} & \frac{264566299}{435891456000} & -\frac{171220639}{58118860800} \end{pmatrix};$$

$$B_1 = \begin{pmatrix} \frac{450855749083}{762810048000} & \frac{193289207}{1482624000} & -\frac{103627613}{2594592000} & \frac{119702819}{8717829120} \\ \frac{1005044731}{2905943040} & \frac{294593723}{486486000} & \frac{261825097}{3459456000} & -\frac{119892569}{7264857600} \\ -\frac{7382527}{290594304} & \frac{3912369061}{10378368000} & \frac{294593723}{486486000} & \frac{215857459}{4843238400} \\ \frac{485715409}{43589145600} & -\frac{104898883}{2594592000} & \frac{610887817}{1482624000} & \frac{454827967333}{762810048000} \end{pmatrix};$$

$$B_2 = \begin{pmatrix} -\frac{2891921}{717516800} & \frac{128312183}{145297152000} & -\frac{81674251}{653837184000} & \frac{25797689}{3051240192000} \\ \frac{345704453}{87178291200} & -\frac{27037529}{34871316480} & \frac{74011757}{726485760000} & -\frac{133787}{20432412000} \\ -\frac{49253033}{7264857600} & \frac{11344999}{10461394944} & -\frac{110821937}{871782912000} & \frac{5512813}{726485760000} \\ \frac{249792089}{9686476800} & -\frac{37865123}{14529715200} & \frac{326587901}{1307674368000} & -\frac{11591303}{871782912000} \end{pmatrix};$$

$$D_1 = \begin{pmatrix} -\frac{184329877}{660441600} & 0 & 0 & 0 \\ 0 & -\frac{109551893}{471744000} & 0 & 0 \\ 0 & 0 & -\frac{92427157}{471744000} & 0 \\ 0 & 0 & 0 & -\frac{109551893}{660441600} \end{pmatrix}$$

It is $A_{1,1}$-stable and can be implemented with one additional initial and final block equations from (3.16) and (3.18) respectively.

4 Application of Second Derivative MB$_2$VMs on Amenable Differential Algebraic Equations

One of the advantages of second derivative MB$_2$VMs in (3.20) is that, they can easily be extended to the solution of differential algebraic equations. In fact, different form of DAEs can be expressed in the form

$$M\frac{dt}{dx} = f(x, t) \tag{4.1}$$

where,

$$M = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 0 & \vdots \\ & \ddots & \ddots & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 \\ 0 & \cdots & 0 & \cdots & 0 \end{pmatrix} \tag{4.2}$$

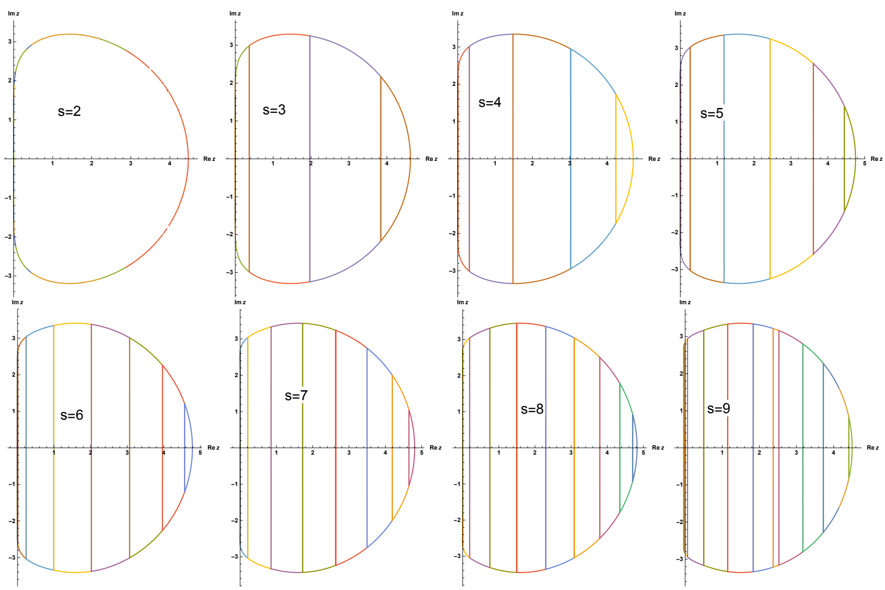

Figure 1: Boundary loci of the MBGSDLMME in (3.4) of order $p = s(k+1)$ for $k = 2$, $s = 2(1)9$; $D_{u,1}$.

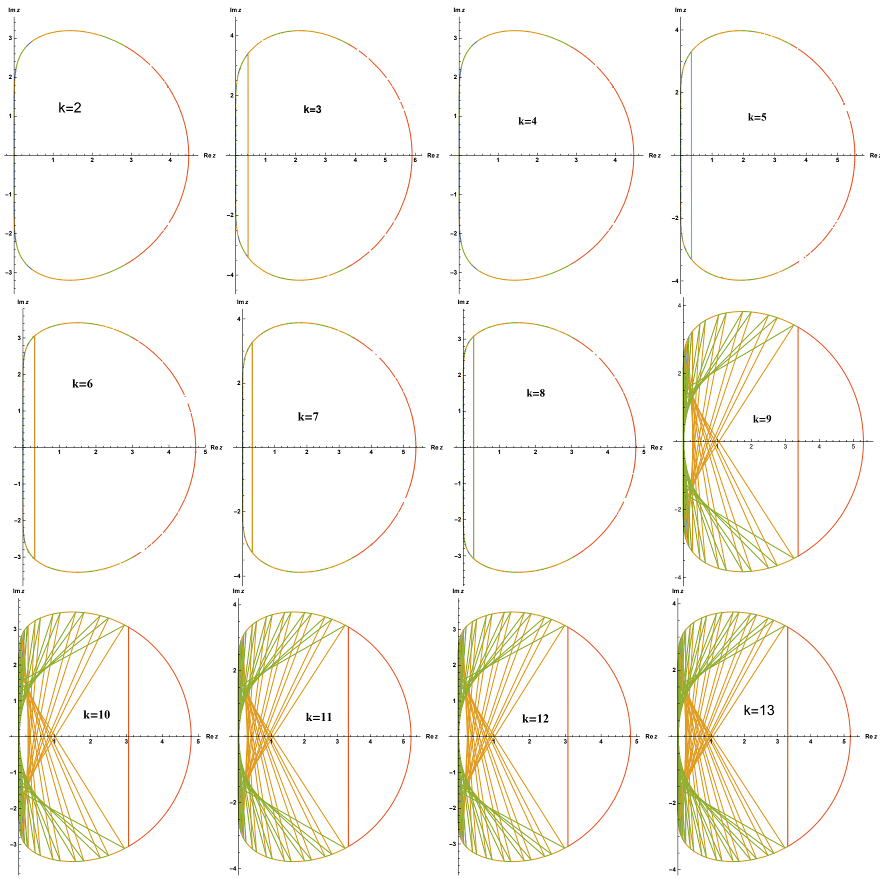

Figure 2: Boundary loci of the MBGSDLMME in (3.4) of order $p = s(k+1)$ for $s = 2$, $k = 2(1)13$; $D_{u,1}$.

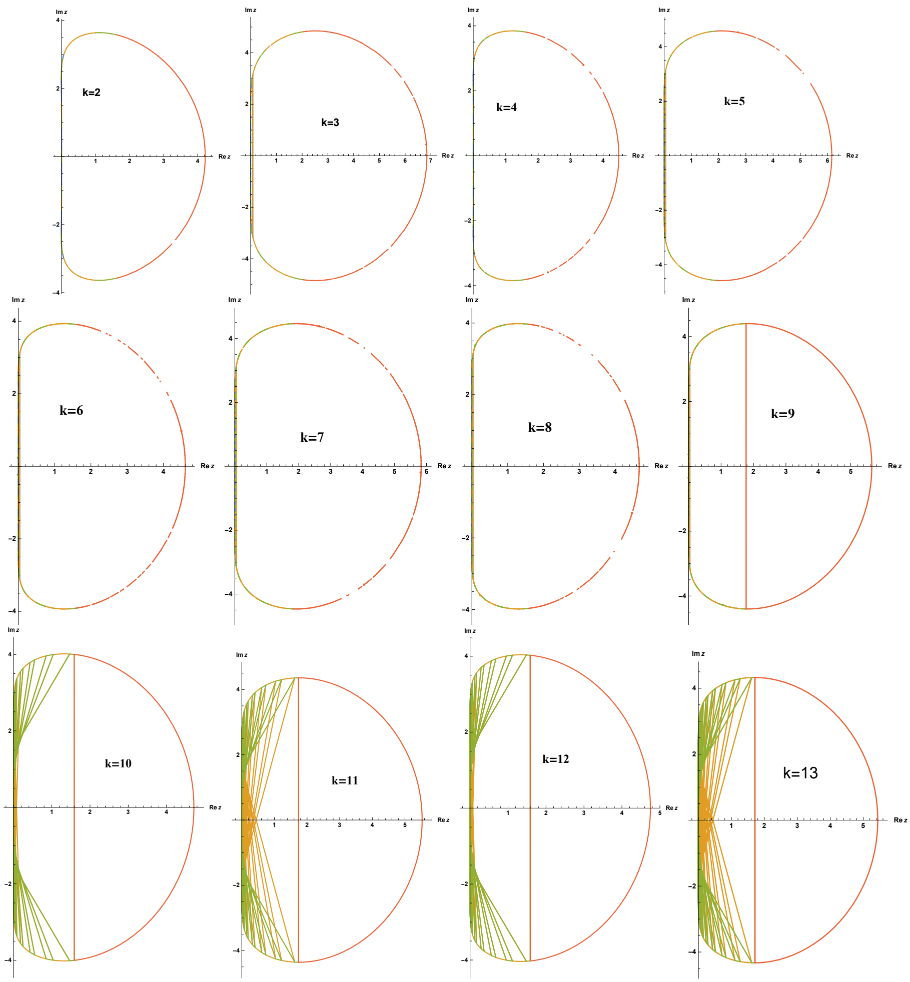

Figure 3: Boundary loci of the MBGSDLMME in (3.4) of order $p = s(k+1)$ for $s = 2$, $k = 2(1)13$; $D_{u,2}$.

is singular. Many special classes of problems are naturally represented in DAEs forms such as mechanical systems and systems of rigid bodies (Hairer and Wanner 1996, p. 463; Brenan et al. 1989, p. 130), electric networks (Brenan et al. 1989, p. 170), multibody and constrained Hamiltonian systems (Hairer and Wanner 1996,p. 530). The DAE in (4.1) can be converted to ODEs in (1.2) through repeated analytic differentiation.This leads to the following definition.

Definition 4.1. cf: [16] The non-linear DAEs

$$f\left(t'(x), t(x), x\right) = 0, \tag{4.3}$$

has index μ, if μ is the minimal number of differentiation,

$$f\left(t'(x), t(x), x\right) = 0, \frac{df\left(t'(x), t(x), x\right)}{dx} = 0, \cdots, \frac{d^{\mu} f\left(t'(x), t(x), x\right)}{dx^{\mu}} = 0, \tag{4.4}$$

where (4.4) gives room to extract an explicit system of ordinary differential equations $g'(x) = \varphi(t(x), x)$.

The following DAEs,

$$\begin{array}{c|c|c|c} (a) \quad \begin{aligned} t' &= f(x,t) \\ 0 &= g(x,t) \end{aligned} & (b) \quad \begin{aligned} t' &= f(x,t) \\ 0 &= g(x,t,z) \end{aligned} & (c) \quad \begin{aligned} t' &= f(x,t,z) \\ 0 &= g(x,t,z) \end{aligned} & (d) \quad \begin{aligned} x' &= f(x,t,z) \\ 0 &= g(x,t) \end{aligned} \end{array} \tag{4.5}$$

are amenable to be solved by second derivative MB_2VM. The (a) does not contain algebraic variables in both the differential equation and algebraic equation part and (b) does not contain algebraic variables in the differential equation part. However, the (c) in (4.5) is solvable by $SDMB_2VM$, if it is feasible to make the algebraic variables z the subject of relation in the algebraic equation part. While the DAE of the form in (d) is not amenable to be solved by second derivative MB_2VMs in general. Note that, there are algebraic variables z in the differential part, but absent in the algebraic constraint. In fact, the first derivative of the algebraic variables z can not be obtained from the differential part. On account of this, (d) is not amenable to be solved by second derivative methods except an explicit z' is provided, see, [23] pp.336 and [35] for example of (d). By applying the MBGSDLMME in (3.20) on (a) in (4.5) gives

$$\begin{aligned}\bar{A}_N\bar{Y}_{n+1} + \bar{A}_0\bar{Y}_n = h\left(\bar{B}_N\bar{F}(Y_{n+1}, Z_{n+1}) + \bar{B}_0\bar{F}(Y_n, Z_n)\right) \\ + h^2\left(\bar{D}_N\bar{F}'(Y_{n+1}, Z_{n+1}) + \bar{D}_0\bar{F}'(Y_n, Z_n)\right)\end{aligned} \tag{4.6}$$

$$\mathbf{O} = I_N\bar{G}(Y_{n+k}, Z_{n+k}); I_N = (I_s, I_s, \cdots, I_s)^T \tag{4.7}$$

The algebraic in (4.7) can also be replaced by

$$\mathbf{O} = \begin{cases} \bar{B}_N{*}\bar{G}(Y_{n+1}, Z_{n+1}) + \bar{B}_0{*}\bar{G}(Y_n, Z_n) \qquad or \\ \\ \bar{G}(Y_{n+k}, Z_{n+k}) + h\bar{D}_N^*\bar{G}'(Y_{n+k}, Z_{n+k}) \end{cases} \tag{4.8}$$

The option 4.7 was consider in the numerical experiment. Here I_N, $\bar{B}_N*$, $\bar{B}_0*$ and $\bar{D}_N*$ are coefficients from a method of the same order as (4.6) to avoid degradation in order of convergences.

5 Numerical Experiment

In this section we present the results of some numerical experiments on some Stiff ODEs, DAEs to illustrate the performance of the MBGSDLMME in (3.4). The MBGSDLMME in (3.32) for $k = 2$, $p = 8$, (i.e MBGSDLMME-8) is implemented as main method in one-block formalism in (3.20) along with two initial block formulas and one final block formula in (3.9) and (3.10) respectively, induced by eight order MBGSDLMME .The iteration scheme we have adopted to use in resolving the implicitness in (3.20) is the Newton-Raphson technique. Thus the multi-block solution $\bar{Y}_{n+1} = \bar{Y}_{n+1}^{[q]}$, in (3.21) is iteratively obtained from,

$$\bar{Y}_{n+1}^{[i+1]} = \bar{Y}_{n+1}^{[i]} - \left(\frac{\partial M(Y_{n+1}^{[i]})}{\partial Y_{n+1}}\right)^{-1} M(Y_{n+1}^{[i]}); \qquad i = 0(1)q \quad q > 1, \tag{5.1}$$

where

$$\frac{\partial F(Y_{n+1})}{\partial Y_{n+1}} = \frac{\partial\left(f_{n+1},\cdots,f_{n+N\cdot s}\right)}{\partial\left(y_{n+1},\cdots,y_{n+N\cdot s}\right)} = \begin{pmatrix} \frac{\partial f_{n+1}}{\partial y_{n+1}} & \frac{\partial f_{n+1}}{\partial y_{n+2}} & \cdots & \frac{\partial f_{n+1}}{\partial y_{n+N\cdot s}} \\ \frac{\partial f_{n+2}}{\partial y_{n+1}} & \frac{\delta f_{n+2}}{\partial y_{n+2}} & \cdots & \frac{\partial f_{n+2}}{\partial y_{n+N\cdot s}} \\ \vdots & & & \\ \frac{\partial f_{n+s}}{\partial y_{n+1}} & \frac{\partial f_{n+s}}{\partial y_{n+2}} & \cdots & \frac{\partial f_{n+N\cdot s}}{\partial y_{n+N\cdot s}} \end{pmatrix}. \quad (5.2)$$

and

$$\frac{\partial F'(Y_{n+1})}{\partial Y_{n+1}} = \frac{\partial\left(f'_{n+1},\cdots,f'_{n+N\cdot s}\right)}{\partial\left(y_{n+1},\cdots,y_{n+N\cdot s}\right)} \quad (5.3)$$

$$M(Y_{n+1}) = \bar{A}_N\bar{Y}_{n+1} + \bar{A}_0\bar{Y}_n - h\bar{B}_0\bar{F}_n - h\bar{B}_N\bar{F}_{n+1} - h^2\bar{D}_0\bar{F}'_n - h^2\bar{D}_N\bar{F}'_{n+1} = 0. \quad (5.4)$$

A modified Newton-Raphson method which uses a fixed Jacobian $J = \frac{\partial M}{\partial Y}$ from the ODEs in (1.2) and (4.1) when available can also be employed. The method in (3.20) are implemented with minimum block size using the Newton-Raphson method in (5.1).

Problem 1: Consider the linear problem in [23]

$$y' = \begin{pmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \quad (5.5)$$

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

This system of ODEs is stiff with the stiffness ratio $S = 28.5$ and the eigenvalues of the Jacobian matrix are $\lambda_1 = -2$ and $\lambda_{2,3} = -40 + 40i$. Table 1 contains the maximum relative error $\max_{1<i<3} \mid y_i(x) - y_{i,h} \mid /(1+ \mid y_{i,h} \mid)$ in the interval $0 < x \leq 1$ using MBGSDLMME-8. The performance compares with generalized backward differentiation formulas (GBDFs) of order $p = 8$, Extended Trapeziodal rule of first kind (ETR) of order $p = 8$ and Extended Trapeziodal rule of second kind (ETR_2s) of order $p = 8$ in [23]. It is observed that the MBGSDLMME-8 perform better than the GBDFs, ETR and ETR_2s, where rate is the numerical order of convergence given in bracket and is computed from

$$rate = log_2\left(\frac{T_1}{T_2}\right); \quad i = 1(1)m, \quad m = 3, \quad 0 < x \leq 1$$

$$T_1 = \max_{1<i<3} \mid y_i(x) - y_{i,h} \mid /(1+ \mid y_{i,h} \mid) \tag{5.6}$$

$$T_2 = \max_{1<i<3} \mid y_i(x) - y_{i,\frac{h}{2}} \mid /(1+ \mid y_{i,\frac{h}{2}} \mid)$$

This rate in Table 1 is obtained from applying the MBGSDLMME-8 with two different step sizes h and $\frac{h}{2}$. From which the rate is computed from the log of the absolute value of the ratio of two errors at the output point x. Here $y_i(x)$ is the exact solution at x since it is available for the ordinary differential equations in Problem 1. The numerical order of convergence conform with the theoretical order.

Problem 2: Consider the Lorenz system

$$\begin{aligned} y_1'(x) &= b(y_2(t) - y_1(t)) \qquad & y_1(0) = 1 \\ y_2'(x) &= -y_1y_3 + ay_1 - y_2(t) \qquad & y_2(0) = 5 \\ y_3'(x) &= y_1(t)y_2(t) - cy_3(t) \qquad & y_3(0) = 10 \end{aligned} \tag{5.7}$$

The plot is given in Figures 4, 5 and 6 for values of $a = 28$, $b = 10$, $c = \frac{8}{3}$.

In Figure 4, is the time series plot of individual $y_1(t)$, $y_2(t)$, $y_3(t)$ against time t. The portrait of $y_2(t)$ against $y_1(t)$, $y_3(t)$ against $y_2(t)$ and $y_3(t)$ against $y_1(t)$ is given in Figure 5, while the three-dimensional space plot is shown in Figure 6.

Problem 3: The problem consider is chemical rection kinetics of index 1 in [16]

$$\begin{aligned} &y_1' = -0.04y_1 + 10^4y_2y_3, \quad y_2' = 0.04y_1 - 10^4y_2y_3 - 3\times 10^7 y_2^2, \\ &0 = y_1 + y_2 + y_3 - 1; \quad y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0. \end{aligned} \tag{5.8}$$

From definition (4.1), the DAE of index one in problem 3 can be written in ODEs in (1.2) as,

Problem 4: Robertson's equation, [16]

$$\begin{gathered} y_1' = -0.04y_1 + 10^4 y_2 y_3, \quad y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2, \\ y_3' = 3 \times 10^7 y_2^2; \quad y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0. \end{gathered} \tag{5.9}$$

The problem considered in (5.8) aand (5.9). Table 2, contains the absolute error which is given as the modulus of the ODE15s in MATLAB minus the numerical solution of the MBGSDLMME.

Problem 5: The next problem is of index one, [23, 40]

$$\begin{pmatrix} 1 & -x & x^2 \\ 0 & 1 & -x \\ 0 & 0 & 0 \end{pmatrix} y' + \begin{pmatrix} 1 & -(x+1) & x+x^2 \\ 0 & -1 & x-1 \\ 0 & 0 & 1 \end{pmatrix} y = \begin{pmatrix} 0 \\ 0 \\ sin(x) \end{pmatrix} \tag{5.10}$$

with boundary condition $y_1(0) = 1$ and $y_2(1) - y_3(1) = e$. The theoretical result is

$$y_1 = e^{-x} + xe^x, \quad y_2 = e^x + xsin(x), \quad y_3 = sin(x)$$

suppose y_3' is written as $\epsilon y_3'$, then the DAE in (5.10) transforms to

$$y' + \begin{pmatrix} 1 & -2x-1 & x^2 + (x-1)x + x \\ 0 & -1 & \frac{x}{\varepsilon} + x - 1 \\ 0 & 0 & \frac{1}{\varepsilon} \end{pmatrix} y = \begin{pmatrix} 0 \\ \frac{xsin(x)}{\varepsilon} \\ \frac{sin(x)}{\varepsilon} \end{pmatrix} \tag{5.11}$$

this problem (5.11) is excessively stiff and sensitive to the solution from the third component due to the parameter $\varepsilon \to 0$. This readily explains why ODE15s is unable to give a solution of reasonable accuracy compared to the exact solution and the solution from MBGSDLMME-8. However, ODE15s is considered as a reference solution.

Table 1: Numerical solution of problem 1 in the interval $0 < x \leq 1$ with $Ns = (N \cdot s)^* = 4$.

	MBGSDLMME-8	GBDF-8	ETR-8	ETR_2-8s
$(N \cdot s)^*$	4	8	8	8
steps	error (rate)	error (rate)	error (rate)	error (rate)
50	$3.32e-5$ (−)	$7.32e-2$ (−)	$1.47e-3$ (−)	$1.30e-3$ (−)
100	$1.63e-7$ (7.50)	$4.49e-4$ (7.31)	$7.81e-6$ (7.56)	$6.72e-6$ (7.60)
200	$1.05e-9$ (7.30)	$2.68e-6$ (7.39)	$4.88e-8$ (7.32)	$4.20e-8$ (7.32)
400	$4.76e-12$ (7.99)	$1.54e-8$ (7.45)	$1.84e-10$ (7.59)	$1.54e-10$ (8.09)

The maximum relative error from Ode15s at $x = 1$ is $3.660087954199254e-5$

Table 2: Comparison of results from problem 3, 4 using $Erry_i =\mid y_i\,(3.20) - ODE15s(y_i) \mid, i = 1(1)3,\ h = 0.0001$.

	Problem 3			problem 4		
x	$Erry_1$	$Erry_2$	$Erry_3$	$Erry_1$	$Erry_2$	$Erry_3$
1	$5.18e-6$	$-7.89e-10$	$5.18e-6$	$-4.42e-7$	$-7.04e-11$	$4.4e-7$
5	$1.03e-5$	$1.19e-9$	$1.03e-5$	$-4.19e-6$	$8.50e-10$	$4.19e-6$
10	$6.28e-5$	$5.09e-9$	$6.28e-5$	$2.05e-5$	$2.21e-9$	$2.05e-5$

Table 3: Numerical solution of problem 5 with $Ns = (N \cdot s)^* = 4$, $h = 0.01$.

x	Exact solution $(y_1, y_2, y_3)^T$	MBGSDLMME-8 solution $(y_1, y_2, y_3)^T$	ODE15s solution$(y_1, y_2, y_3)^T$
	3.035898818647817	3.03706392172143	2.662759915698755
1	3.518900191163779	3.51905149198082	3.201941362146939
	0.836025978600521	0.836025978600521	0.788432436870595
	217854.9150401765	217796.8076402711	221498.6357290881
10	21801.94812091745	21796.29119316302	22143.5041602270
	-0.535603334614296	-0.535603334614296	-0.5440211109
	$9.809460533275866e+18$	$9.804702611996597e+18$	$8.239333037971687e+18$
40	$2.449915218100874e+17$	$2.449674714825473e+17$	$2.06761180705137e+19$
	0.717846740396360	0.717846740396360	0.0

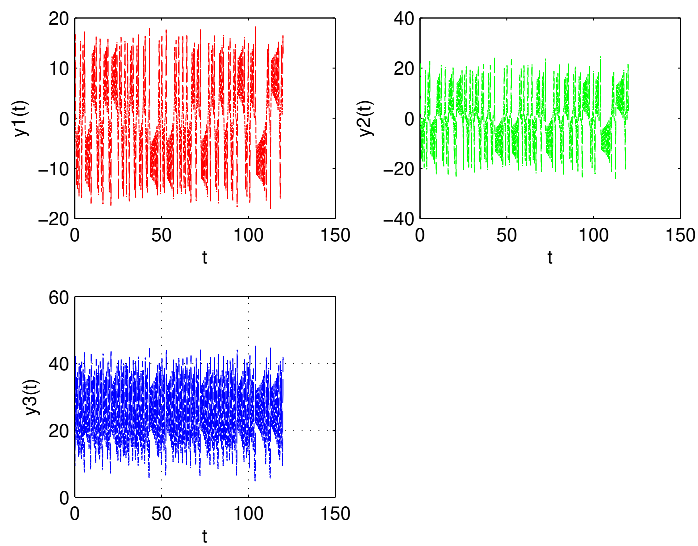

Figure 4: Time series result for the problem in (5.7) when $h = 0.01$.

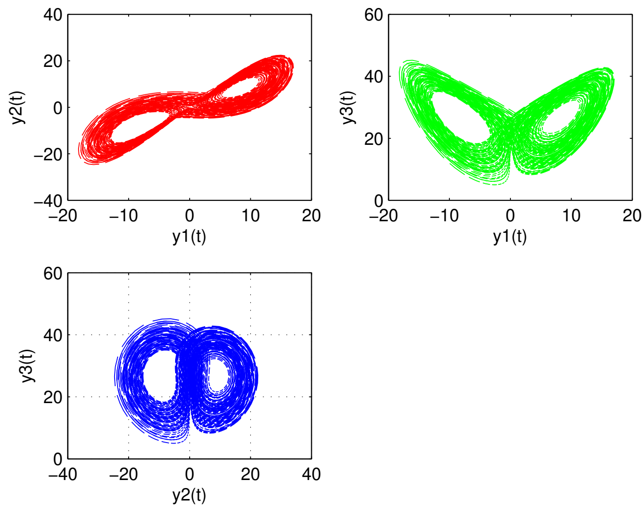

Figure 5: Phase portraits for the Lorenz system in (5.7) when $h = 0.01$.

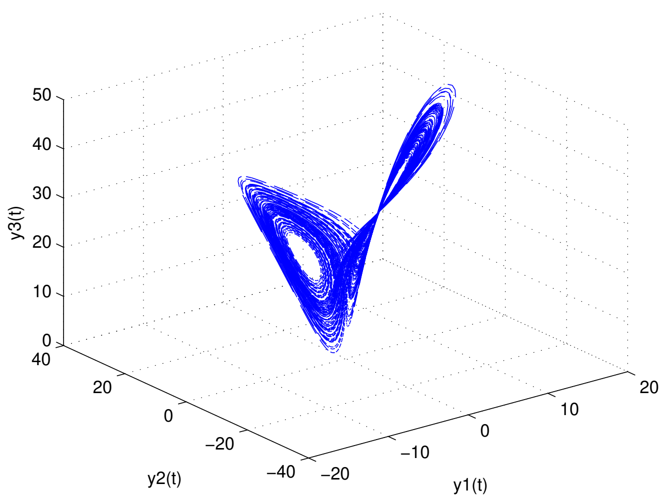

Figure 6: Three-dimensional space for the Lorenz system in (5.7) when $h = 0.01$.

6 Conclusion

This paper considered a very large scale integration methods (VLSIM) in the numerical solution of differential equations. The proposed methods is a new family of multi-block boundary value integration methods based on the Enright type-methods. The theoretical properties of the methods with respect to convergency and stability along with other practical aspect of implementation have also been presented. The Weiner-Hopf matrix factorization of the characteristics matrix polynomial of the main method along with the root distribution of the arising stability polynomial have been used to determine the structure of the arising second derivative multi-block boundary value method in (3.4). Finally, the numerical results presented in Tables 1, 2 and 3 , shows that MBGSDLMME compare in accuracy with methods from [23] and [35] on some considered ODEs and DAEs in Section 5.

Conflict of interest

The authors declare that they have no conflict of interest.

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