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Generalized Enright block methods for Stiff ODEs

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Abstract

A general theoretical background for a class of parallel second derivative methods is introduced. A parallel block generalization of the Enright second derivative block methods are developed and their stabilities are investigated by means of root locus plots. The resultant parallel methods are found to be L–stable for block size $k \leq 6$ ***and are of order (k+2).***

Keywords:
Block methods, stiff initial value problems, parallel methods, stability.

1.0 Introduction

Parallel block methods for solving the stiff initial value problem

$$y' = f(y),\ y(x_0) = \alpha \tag{1.1}$$

are developed. The idea of block method is believed to have originated from Milne's book [3, 12], where a method to generate starting values for a multi step method is discussed. Watts and Shampine [18] used the idea when they considered implicit block methods. An early notable work dedicated to parallel block methods are those of Birta and Abou–Rabia [1, 3], and of Chu and Hamilton [5].

Chu and Hamilton [5] introduced multi–block methods, Houwen and Sommeijer [9] developed block Runge–Kutta methods, Voss and Abbas [17] considered block predictor – corrector schemes, Omarjid [15] developed block methods based on Adams type formulas, Zarina et al [20] implemented a variable step size block methods based on Backward differentiation type methods, Yahaya and Kumleng [19] developed a block method that stabilizes Simpson's method, Muka and Ikhile [13] also stabilized Simpson's method by means of employing second derivative in a parallel block method.

Zarina et al [20] observed that most block methods developed are only suitable for non stiff ODEs. The work of Yahaya and Kumleng [19] shows that Block methods can be used to improve the stability of methods adjudged unstable when used alone. This is achieved by adjoining a LMM in block form to make the resultant method to become stable. We are motivated to develop a class of block methods that are not only suitable for stiff ODEs but in addition are *L*–stable. Dalhquist order barrier places a very severe restriction on Linear Multi step Methods [8, 11]. One way of circumventing this barrier is to introduce the second derivative as done in Enright [6] and Chakravarti and Kamel [4]. Zarina et al [20] were able to

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achieve their aim by developing block methods based on backward differentiation method. Backward differentiation methods are known to be suitable for mildly stiff ODEs. In the spirit of Enright [6], we develop block methods with second derivatives.

The paper is organized as follows in Section 2 we consider the basic theory of the second derivative block method, in Section 3 we introduce the Generalized Enright block methods, Section 4 stability analysis of Generalized Enright block method is done using the root locus plot [10], in section 5 numerical experiment.

2.0 Parallel second derivative block methods

***Definition* 2.1**

Let y_{n+i} denote a numerical approximation to the exact solution values $y(x_n + ih)$, and Let $Y_{n+1} = (y_{n+1}, y_{n+2}, ..., y_{n+k})$ and $Y_n = (y_{n-k+1}, y_{n-k+2}, ..., y_n)$, also let a block of second derivative be defined as $F'(Y_{n+1}) = (f'_{n+1}, f'_{n+2}, ..., f'_{n+k})$ and $F'(Y_n) = (f'_{n-k+1}, f'_{n-k+2}, ..., f'_n)$. A one block k-point second derivative method of our interest is defined by the recurrence relation

$$Y_{n+1} = AY_n + hBF(Y_n) + hDF(Y_{n+1}) + h^2EF'(Y_n) + h^2GF'(Y_{n+1}) \qquad (2.1)$$

where A,B,D,E,G are $k \times k$ matrices with real entries. The elements are carefully chosen with stability and accuracy requirement in mind. $F(Y_{n+1})$ *and* $F'(Y_{n+1})$ are vectors with components $f(y_{n+j})$ *and* $f'(y_{n+j})$, $j = 1,2,\ldots,k$ respectively. Our aim is to develop methods from (2.1) that are A–stable which are implementable on parallel processors. In order to achieve the later the block need be parallelizable [3, 16]. Methods whose blocks are parallelizable are often explicit. Implicit block methods are easily parallelizable if their implicit co-efficient blocks are diagonal. For this reason we set matrices D and G in (2.1) to be diagonal.

3.0 Generalized Enright block methods: Parallelization of Enright [6] second derivative sequential method

Based on the nature of matrices A, B, D, E, and G, parallel second derivative block methods that have computational complexities which compare with traditional LMMs can be developed. Note that second derivative parallel block backward differentiation type formulas (SDBDF) developed in [14] are of the form in (2.1) with matrices B and E set to zero. In this section, parallel block methods of generalized Enright methods are developed. Enright [6] considered the following class of second derivative LMMs

$$y_{n+1} = \sum_{r=1}^{k} \alpha_r y_{n+1-r} + h\sum_{r=0}^{k} \beta_r f_{n+1-r} + h^2 \sum_{r=0}^{k} \gamma_r f'_{n+1-r}. \qquad (3.1)$$

Enright in an attempt to get methods that are stiffly–stable, re-model (3.1) as

$$y_{n+1} = y_n + h\sum_{r=0}^{k} \beta_r f_{n+1-r} + h^2 \gamma_0 f'_{n+1}. \qquad (3.2)$$

If we set k = 1in (3.2), then

$$y_{n+1} = y_n + h\beta_1 f_n + h\beta_0 f_{n+1} + h^2 \gamma_0 f'_{n+1}; \qquad (3.3)$$

which is the simplest form of zero stable Enright's methods. Block equivalent of (3.2) is therefore

$$Y_{n+1} = AY_n + hBF(Y_n) + hDF(Y_{n+1}) + h^2GF'(Y_{n+1}) \qquad (3.4)$$

Observe that matrix E in (2.1) has been set to zero. Also, matrix A in (3.4) is k x k matrix with zero elements except at the last column *i.e*

$$A=\begin{pmatrix}0&0&\cdots&0&1\\0&0&\cdots&0&1\\0&0&\cdots&0&1\\\vdots&\vdots&\ddots&\vdots&\vdots\\0&0&\cdots&0&1\end{pmatrix}$$

D and *G* are diagonal matrices. The elements of matrices *A, B, D* and *G* are determined using the Taylor expansion method and the method of undetermined coefficients.

***Lemma* 3.1**

Let $e = [1,1,1,...,1]T$, and $c = [1,2,3,..,k]T$ and let us define

$$C_j = jDc^{j-1} - jB(c-ke)^{j-1} + j(j-1)Gc^{j-2} - c^j,\ j=1,2,3,... \tag{3.5}$$

A one block *k*-point second derivative method as given in (3.4) is of order *p*, if $C_j = 0, C_{p+1} \neq 0$ for j = 1, 2,...,*p*.

In order to compare the components of error vectors of methods (3.2) with the error constants corresponding to conventional linear multistep methods, we shall adopt the normalized error vectors as introduced by Sommeijer et al [16], and extended to the class of block methods in (3.4). For methods (3.4) the normalized error vectors is given as

$$E_j = \frac{C_j}{(j-1)!(j(B+D)+G)e}; \qquad j = p+1. \tag{3.6}$$

Division is done component wise. The proposed Generalized Enright block methods (GEBM) are given as follows, after solving the arising order conditions $C_j = 0,\ j = 1,2,\cdots,p$ in (3.5).

For *k* = 2, order *p* = 4

$$B=\begin{pmatrix}-\frac{1}{48}&\frac{5}{12}\\-\frac{4}{27}&1\end{pmatrix}, D=\begin{pmatrix}\frac{29}{48}&0\\0&\frac{31}{27}\end{pmatrix}\quad G=\begin{pmatrix}-\frac{1}{8}&0\\0&-\frac{4}{9}\end{pmatrix} \tag{3.7}$$

with $C_5 = \begin{bmatrix}\frac{7}{1440} & \frac{1}{10}\end{bmatrix}^T,\ E_5 = \begin{bmatrix}\frac{7}{168480} & \frac{9}{20160}\end{bmatrix}^T$

For *k* = 3, order *p* = 5

$$B=\begin{pmatrix}\frac{7}{1080}&-\frac{1}{20}&\frac{19}{40}\\\frac{3}{40}&-\frac{56}{135}&\frac{13}{10}\\\frac{297}{1000}&-\frac{27}{20}&\frac{103}{40}\end{pmatrix}, D=\begin{pmatrix}\frac{307}{540}&0&0\\0&\frac{1123}{1080}&0\\0&0&\frac{739}{500}\end{pmatrix}\quad G=\begin{pmatrix}-\frac{19}{180}&0&0\\0&-\frac{31}{90}&0\\0&0&-\frac{69}{100}\end{pmatrix} \tag{3.8}$$

$C_6 = \begin{bmatrix}\frac{17}{7200} & \frac{13}{225} & \frac{333}{800}\end{bmatrix}^T,\ E_6 = \begin{bmatrix}\frac{17}{5092800} & \frac{13}{314700} & \frac{37}{184640}\end{bmatrix}^T$

For *k* =4, order *p* = 6

$$B=\begin{pmatrix}-\frac{17}{5760}&\frac{1}{45}&-\frac{41}{480}&\frac{47}{90}\\-\frac{52}{1125}&\frac{7}{24}&-\frac{4}{5}&\frac{143}{90}\\-\frac{37}{160}&\frac{162}{125}&-\frac{1863}{640}&\frac{7}{2}\\-\frac{320}{441}&\frac{56}{15}&-\frac{2752}{375}&\frac{298}{45}\end{pmatrix}, D=\begin{pmatrix}\frac{3133}{5760}&0&0&0\\0&\frac{2897}{3000}&0&0\\0&0&\frac{21539}{16000}&0\\0&0&0&\frac{10466}{6125}\end{pmatrix}, G=\begin{pmatrix}-\frac{3}{32}&0&0&0\\0&-\frac{43}{150}&0&0\\0&0&-\frac{441}{800}&0\\0&0&0&-\frac{464}{525}\end{pmatrix} \tag{3.9}$$

$$C_7=\left[\frac{41}{30240}\quad\frac{359}{9450}\quad\frac{1737}{5600}\quad\frac{7016}{4725}\right]^T,\ E_7=\left[\frac{41}{150368400}\quad\frac{359}{93305520}\quad\frac{193}{9304400}\quad\frac{877}{11531160}\right]^T$$

For k = 5, order p = 7

$$B=\begin{pmatrix} \frac{41}{25200} & -\frac{529}{40320} & \frac{373}{7560} & -\frac{1271}{10080} & \frac{2837}{5040} \\ \frac{359}{11340} & -\frac{8}{35} & \frac{151}{210} & -\frac{3704}{2835} & \frac{787}{420} \\ \frac{5211}{27440} & -\frac{1417}{1120} & \frac{4941}{1400} & -\frac{23463}{4480} & \frac{2539}{560} \\ \frac{877}{1260} & -\frac{67328}{15435} & \frac{10544}{945} & -\frac{22784}{1575} & \frac{2963}{315} \\ \frac{158125}{81684} & -\frac{124375}{10752} & \frac{228125}{8232} & -\frac{591875}{18144} & \frac{5935}{336} \end{pmatrix},\ D=\begin{pmatrix} \frac{317731}{604800} & 0 & 0 & 0 & 0 \\ 0 & \frac{1721}{1890} & 0 & 0 & 0 \\ 0 & 0 & \frac{1371271}{1097600} & 0 & 0 \\ 0 & 0 & 0 & \frac{1452137}{926100} & 0 \\ 0 & 0 & 0 & 0 & \frac{240206005}{128024064} \end{pmatrix}$$

$$G=\begin{pmatrix} -\frac{863}{10080} & 0 & 0 & 0 & 0 \\ 0 & -\frac{47}{189} & 0 & 0 & 0 \\ 0 & 0 & -\frac{3627}{7840} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1598}{2205} & 0 \\ 0 & 0 & 0 & 0 & -\frac{262775}{254016} \end{pmatrix} \qquad (3.10)$$

$$C_8=\left[\frac{731}{846720}\quad\frac{179}{6615}\quad\frac{7713}{31360}\quad\frac{8608}{6615}\quad\frac{17375}{3456}\right]^T$$

$$E_8=\left[\frac{731}{3377439072\ \ 0}\quad\frac{179}{525142800}\quad\frac{857}{413353920}\quad\frac{269}{32584545}\quad\frac{4865}{190039008}\right]^T$$

For k = 6, p = 8

$$B=\begin{pmatrix} -\frac{731}{725760} & \frac{179}{20160} & -\frac{5771}{161280} & \frac{8131}{90720} & -\frac{13823}{80640} & \frac{12079}{20160} \\ -\frac{358}{15435} & \frac{307}{1620} & -\frac{1076}{1575} & \frac{1801}{1260} & -\frac{5494}{2835} & \frac{2719}{1260} \\ -\frac{23139}{143360} & \frac{136539}{109760} & -\frac{18523}{4480} & \frac{6129}{800} & -\frac{303399}{35840} & \frac{12727}{2240} \\ -\frac{17216}{25515} & \frac{6257}{1260} & -\frac{239488}{15435} & \frac{74672}{2835} & -\frac{1600}{63} & \frac{577}{45} \\ -\frac{4865}{2304} & \frac{4889375}{326592} & -\frac{5749375}{129024} & \frac{6994375}{98784} & -\frac{8991875}{145152} & \frac{105275}{4032} \\ -\frac{2106}{385} & \frac{1053}{28} & -\frac{4844}{45} & \frac{90963}{560} & -\frac{226638}{1715} & \frac{6891}{140} \end{pmatrix}$$

$$D=\begin{pmatrix} \frac{247021}{483840} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{267791}{308700} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{41250539}{35123200} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{7301603}{5000940} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{888252815}{512096256} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{5439943}{2716560} \end{pmatrix}$$

$$B=\begin{pmatrix} -\frac{731}{725760} & \frac{179}{20160} & -\frac{5771}{161280} & \frac{8131}{90720} & -\frac{13823}{80640} & \frac{12079}{20160} \\ -\frac{358}{15435} & \frac{307}{1620} & -\frac{1076}{1575} & \frac{1801}{1260} & -\frac{5494}{2835} & \frac{2719}{1260} \\ -\frac{23139}{143360} & \frac{136539}{109760} & -\frac{18523}{4480} & \frac{6129}{800} & -\frac{303399}{35840} & \frac{12727}{2240} \\ -\frac{17216}{25515} & \frac{6257}{1260} & -\frac{239488}{15435} & \frac{74672}{2835} & -\frac{1600}{63} & \frac{577}{45} \\ -\frac{4865}{2304} & \frac{4889375}{326592} & -\frac{5749375}{129024} & \frac{6994375}{98784} & -\frac{8991875}{145152} & \frac{105275}{4032} \\ -\frac{2106}{385} & \frac{1053}{28} & -\frac{4844}{45} & \frac{90963}{560} & -\frac{226638}{1715} & \frac{6891}{140} \end{pmatrix}$$

$$D=\begin{pmatrix} \frac{247021}{483840} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{267791}{308700} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{41250539}{35123200} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{7301603}{5000940} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{888252815}{512096256} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{5439943}{2716560} \end{pmatrix}$$

$$G=\begin{pmatrix} -\frac{275}{3456} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1466}{6615} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{50319}{125440} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{2446}{3969} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{880825}{1016064} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{113}{98} \end{pmatrix} \qquad (3.11)$$

$$C_9=[\frac{8563}{14515200} \quad \frac{16159}{793800} \quad \frac{255033}{1254400} \quad \frac{116716}{99225} \quad \frac{20085125}{4064256} \quad \frac{164187}{9800}]^T$$

$$E_9=[\frac{8563}{5220706176\ 000} \quad \frac{16159}{5690151936\ 00} \quad \frac{28337}{1494779328\ 00} \quad \frac{29179}{3539037600\ 0} \quad \frac{803405}{2892850652\ 16} \quad \frac{18243}{232019200}]^T$$

For $k = 7$, $p = 9$

$$B=\begin{pmatrix} \frac{8563}{12700800} & -\frac{35453}{5443200} & \frac{86791}{3024000} & -\frac{2797}{36288} & \frac{157513}{1088640} & -\frac{133643}{604800} & \frac{1147051}{1814400} \\ \frac{64636}{3347505} & -\frac{21097184}{117162675} & \frac{136825387}{180765270} & -\frac{477441968}{251062875} & \frac{4300607}{1339002} & -\frac{330119024}{90382635} & \frac{302038697}{100425150} \\ \frac{28337}{201600} & -\frac{440397}{358400} & \frac{148311}{31360} & -\frac{2343}{224} & \frac{1623159}{112000} & -\frac{1141047}{89600} & \frac{155607}{22400} \\ \frac{233432}{354375} & -\frac{2125696}{382725} & \frac{77129}{3780} & -\frac{841472}{19845} & \frac{457448}{8505} & -\frac{4867456}{118125} & \frac{240113}{14175} \\ \frac{20085125}{8781696} & -\frac{452785}{24192} & \frac{129761875}{1959552} & -\frac{9510625}{72576} & \frac{36336875}{169344} & -\frac{23530375}{217728} & \frac{2698355}{72576} \\ \frac{18243}{2800} & -\frac{1100952}{21175} & \frac{312093}{1750} & -\frac{21376}{63} & \frac{856413}{2240} & -\frac{302616}{1225} & \frac{26349}{350} \\ \frac{705680311}{43804800} & -\frac{391394213}{3110400} & \frac{879315829}{2090880} & -\frac{250998139}{324000} & \frac{1172117779}{1399680} & -\frac{707101703}{1382400} & \frac{370255269}{259200} \end{pmatrix}$$

$$D=\begin{pmatrix} \frac{1758023}{352800} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{7788049231}{1054464075\ 0} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{125812403}{112896000} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{368139241}{267907500} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2692665845}{1659740544} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{795618377}{42688000} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2405181711\ 2183}{1144882252\ 8000} \end{pmatrix}$$

$$G=\begin{pmatrix} -\frac{33953}{453600} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{25285994}{150637725} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{15947}{44800} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{114362}{212625} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{447325}{598752} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{15151}{15400} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{277583971}{222393600} \end{pmatrix} \qquad (3.12)$$

Note that this method (k = 7, p = 9) is not *A*–stable, see Figure 4.6.

4.0 Stability of the generalized Enright block methods (3.4)

***Definition* 4.1**

When (2.1) is applied to the scalar test equation $y' = \mu y$, μ a complex constant with $\mathrm{Re}(\mu) < 0$, it yields the recurrence $Y_{n+1} = M(z)Y_n$. The matrix $M(z)$ is the amplification matrix and its eigen values the amplification factors.

$$M(z) = (I - zD - z^2G)^{-1}(A + zB + z^2E) \qquad (4.1)$$

***Definition* 4.2**

A k-dimensional block method with matrix A is called zero stable if A^n is uniformly bounded for all n.

***Definition* 4.3**

An r-dimensional block method is called *A*-stable if the spectral radius $\rho(M(z))$ is such that $\rho(M(z)) \le 1$.

***Definition* 4.4**

An r-dimensional block method is called *L*-stable if it is *A*-stable and if it has an amplification matrix with vanishing eigenvalues at infinity i.e

$$\lim_{z\to\infty} M(z) = (I - zD - z^2G)^{-1}(A + zB + z^2E) = 0 \qquad (4.2)$$

Methods (3.4) are zero stable since the eigenvalues of matrix A are zeros and simple unity (it is uniformly bounded). Also, since E is the zero matrix in (3.4), eigenvalues of M(z) will all vanish at infinity. In what follows, we will examine the *A*–stability of method (3.4) using the root locus plot. The root locus of the stability region is given by the set of points determined by $\rho(M(z)) \le 1$.Figures (4.1) – (4.5) are corresponding root locus plots of methods (3.7), (3.8), (3.9), (3.10) and (3.11) respectively. Figure (4.6) is a plot of block size k =7.

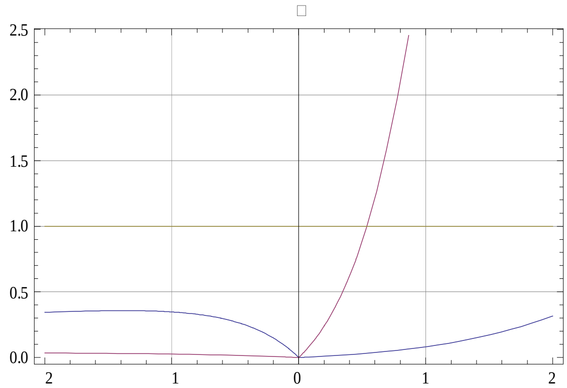

Figure 4.1: Root Locus plot *k = 2*

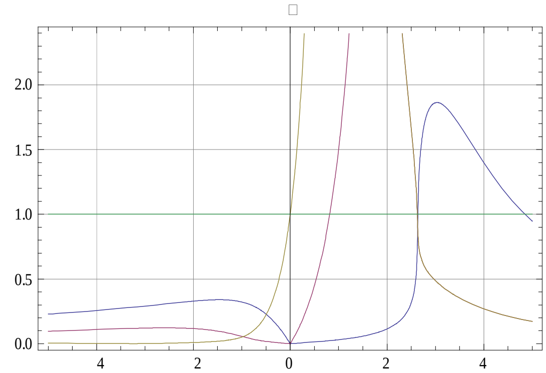

Figure 4.2: Root Locus plot *k = 3*

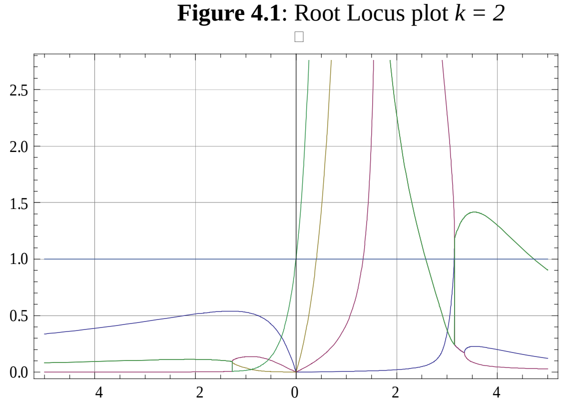

Figure 4.3: Root Locus plot *k=4*

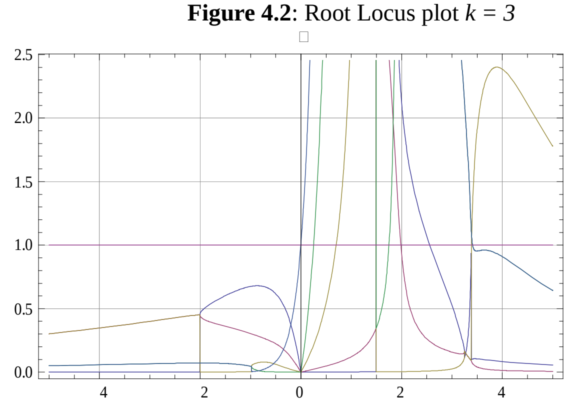

Figure 4.4: Root Locus plot of *k=5*

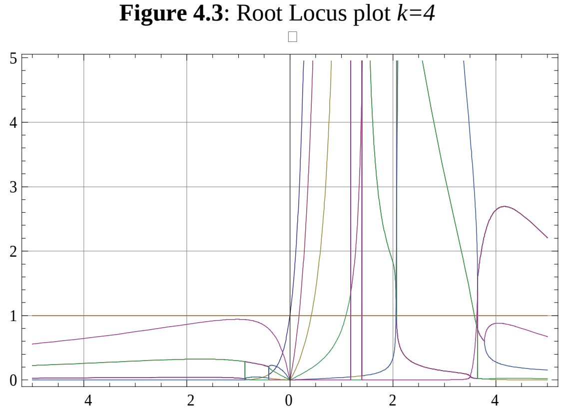

Figure 4.5: Root Locus plot *k = 6*

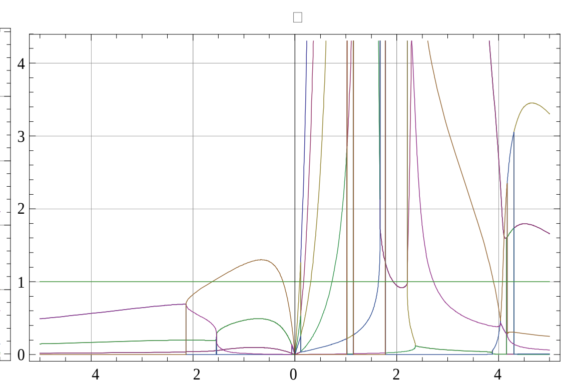

Figure 4.6: Root Locus plot *k = 7*

Observe that spectra radii for block sizes $k \leq 6$ satisfy $|\rho(M(z))| \leq 1$ in the entire left region. Hence, GEBM for block sizes $k \leq 6$ are *L*-stable because of (4.2) while for block sizes $k \geq 7$ GEBM are unstable for stiff IVPs.

5.0 Numerical Experiment

The implicitness of Generalized Enright block methods (GEBM) are resolve using modified Newton–Raphson's technique suggested by Liniger and Willoughby (see [6]), while the starting values are generated using the inverse Euler method $y_{n+1} = y_n + \dfrac{hy_n f_n}{y_n - hf_n}$ given by Fatunla [7]. Consider the stiff initial value problem given in [6], *Problem* 5.1

$$y' = \begin{bmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{bmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} . \tag{5.2}$$

We now present the result obtained by integrating (5.2) using GEBM with block size k =2.

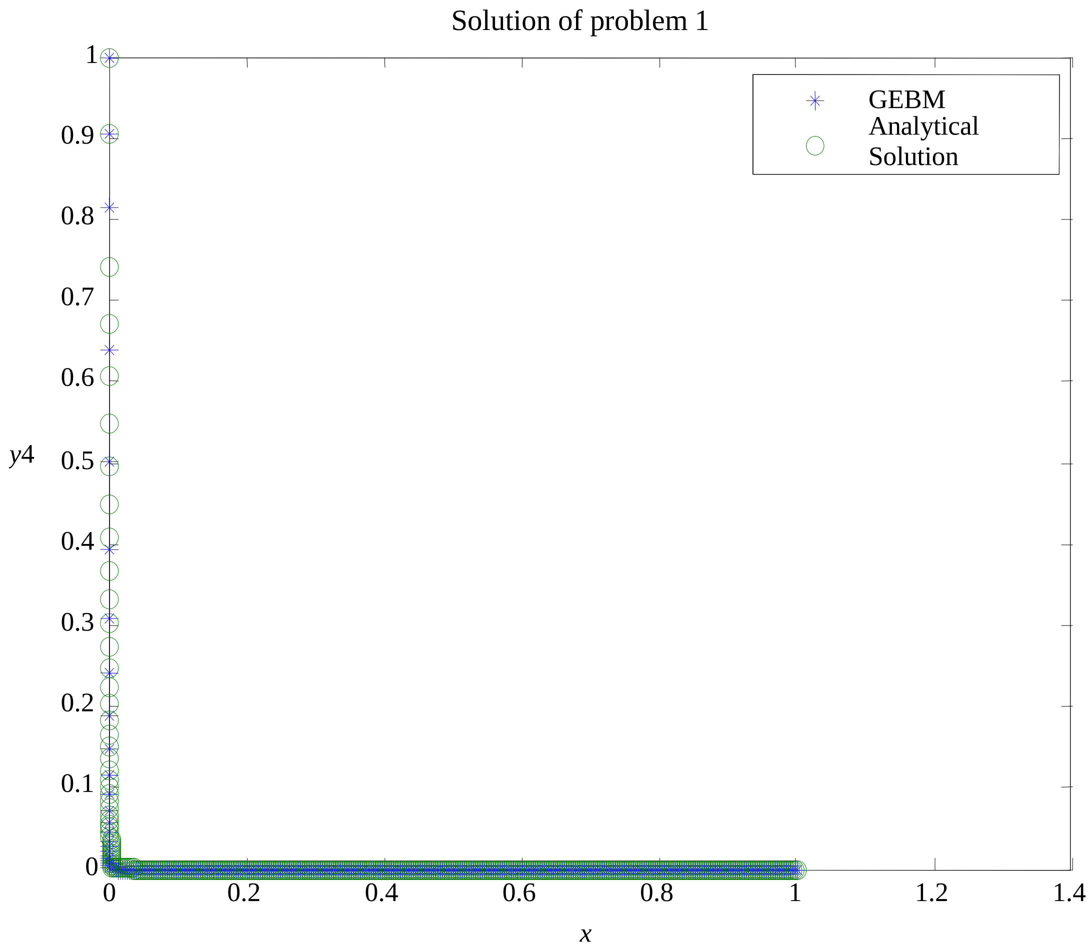

Figure 5.1

The graph in Figure 5.1 shows the accuracy of method (3.4), when compared with the analytical solution of Problem 1. Figure 5.1 shows that the numerical solution is in agreement with the theoretical solution; this made so because of the *L*–stability of the block method.

Conclusively, second derivative block methods have improved stability region compared with sequential second derivative linear multistep methods. GEBM developed in this paper are *L*-stable for block sizes $k \leq 6$ compared with sequential Enright's methods [6] which are *L*–stable for k =2. SDBDF developed in [14] are zero unstable for block size $k \geq 7$, while GEBM are not plagued by zero instability for any step length k.

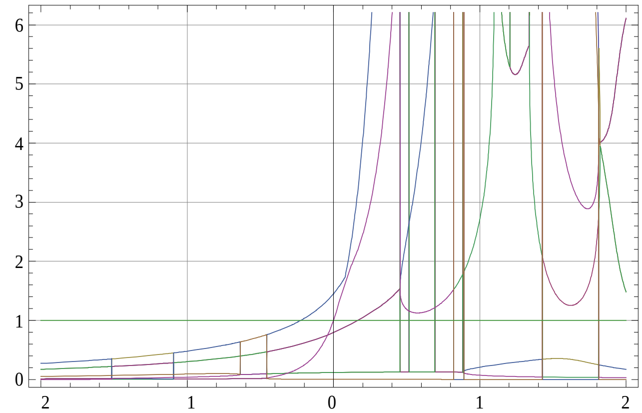

Figure 5.2: *Root Locus plot of SDBDF k = 7*

Compare Figure 5.2 with Figure 4.6. Also, for equal block sizes GEBM have higher order compared to SDBDF. Results presented in Figure 5.1 shows GEBM are suited for integrating stiff initial value problems (1.1); this is true for the *L*–stable methods of block sizes $k \leq 6$.

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