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Second derivative parallel block backward differentiation type formulas for Stiff ODEs

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Abstract

A class of second derivative parallel block Backward differentiation type formulas is developed and the methods are inherently parallel and can be distributed over parallel processors. They are L–stable for block size k ≤ 6 with small error constants when compared to the conventional sequential Linear multi –step methods of the same order. Numerical results are presented.

1.0 Introduction

The interested is to develop numerical methods to solve system of stiff ordinary differential equations of the form

$$y'(x) = Ay(x), \qquad y(x_0) = y_0 \tag{1.1}$$

where $y(x) \in R^n$, A *is an* $n \times n$ real matrix with $\mathrm{Re}(\lambda_i) < 0,\ i = 1,2,\cdots,n.$ λ_i's are the eigenvalues of A. The ratio, $s = \dfrac{\max_i |\mathrm{Re}(\lambda_i)|}{\min_i |\mathrm{Re}(\lambda_i)|}$ is called the stiffness ratio, for s>>1 (1.1) is then said to be stiff see ([4, 7, 8]). As the speed of new generation computers increases, parallel processing gives hope of solving (1.1) faster [12] than using sequential approach. One way of processing (1.1) in parallel is by developing block methods that are essentially parallel in nature; see [1], [6], [11]. High order A–stable or L–stable methods for (1.1) developed are either of block form or sequential methods that incorporate second derivatives to overcome the Dalquist's second order barrier [8]. Among high order A–stable block methods are those developed by Muka and Ikhile [9], Sommeijer et al [12], Yahaya and Kumleng [14], Zarinina et al [15], while sequential second derivative methods include those developed by Cash [2] , Enright [3], Okuonghae and Ikhile [10], Otunta et al [11]. Methods being developed in this paper have characteristics that blend block and second derivative. The paper is organized as follows in Section 2 we consider the basic theory of the method, in section 3 stability analysis of proposed methods are shown using root locus plots, in section 4 we implement the methods.

2.0 The parallel block methods

The methods studied in this paper are block equivalent of second derivative backward differentiation formulas given in Okuonghae and Ikhile [10].

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$$y_{n+k} = \sum_{i=0}^{k-1} \alpha_i y_{n+i} + h\beta_{n+k} f_{n+k} + h^2 \gamma_{n+k} f'_{n+k} \tag{2.1}$$

where h is the step size, f' is the second derivative term. If $\gamma_{n+k} = 0$ then (2.1) is BDF of Gear [5].

***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 $Y_n = (y_{n-k+1}, y_{n-k+2}, ..., y_n)$. A one block k - point second derivative method is defined by the recurrence equation

$$Y_{n+1} = AY_n + hDF(Y_{n+1}) + h^2 GF'(Y_{n+1}) \tag{2.2}$$

where A is $k \times k$ matrix, D and G are $k \times k$ diagonal matrices. $F(Y_{n+1})$ and $F'(Y_{n+1})$ are vectors with components $f(y_{n+j})$ and $f'(y_{n+j})$ respectively, $j = 1,2,..,k$. The elements of matrices A, D and G are determined using the Taylor expansion method and the method of undetermined coefficients.

***Lemma* 2.1**

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

$$C_j = A(c-ke)^j + jDc^{j-1} + j(j-1)Gc^{j-2} - c^j, \; j = 0,1,2,... \tag{2.3}$$

A one block k-point second derivative method as given in (2.2) is of order of consistency p, if for $j = 1,2,..,p$; $C_j = 0$, $C_{p+1} \neq 0$. In order to compare the components of error vectors of methods (2.2) with the error constants corresponding to conventional linear multistep methods, we shall adopt the normalized error vectors as introduced by Sommeijer et al [11], and extended to the class of block methods in (2.2). For methods (2.2) the normalized error vectors is given as

$$E_j = \frac{C_j}{(j-1)!(jD+G)e}; \qquad j = p+1. \tag{2.4}$$

Division is done component wise. The proposed Second derivative parallel block backward differentiation type formulas (SDBDF) are obtained, after solving the arising order conditions $C_j = 0,\ j = 1,2,\cdots,p$ in (2.3). For k =2, order p = 3

$$A = \begin{pmatrix} -\frac{1}{7} & \frac{8}{7} \\ -\frac{8}{19} & \frac{27}{19} \end{pmatrix}, D = \begin{pmatrix} \frac{6}{7} & 0 \\ 0 & \frac{30}{19} \end{pmatrix} \quad G = \begin{pmatrix} -\frac{2}{7} & 0 \\ 0 & -\frac{18}{19} \end{pmatrix} \tag{2.5}$$

with $C_4 = \begin{bmatrix} \frac{1}{21} & \frac{9}{19} \end{bmatrix}^T$, $E_4 = \begin{bmatrix} \frac{1}{396} & \frac{1}{68} \end{bmatrix}^T$

For k =3, order p = 4

$$A = \begin{pmatrix} \frac{4}{85} & -\frac{27}{85} & \frac{108}{85} \\ \frac{27}{115} & -\frac{128}{115} & \frac{216}{115} \\ \frac{864}{1489} & -\frac{3375}{1489} & \frac{4000}{1489} \end{pmatrix}, D = \begin{pmatrix} \frac{66}{85} & 0 & 0 \\ 0 & \frac{156}{115} & 0 \\ 0 & 0 & \frac{2820}{1489} \end{pmatrix} \quad G = \begin{pmatrix} -\frac{18}{85} & 0 & 0 \\ 0 & -\frac{72}{115} & 0 \\ 0 & 0 & -\frac{1800}{1489} \end{pmatrix} \tag{2.6}$$

$$C_5 = \begin{bmatrix} \frac{9}{425} & \frac{144}{575} & \frac{1800}{1489} \end{bmatrix}^T, \; E_5 = \begin{bmatrix} \frac{5}{1066} & \frac{1}{590} & \frac{1}{164} \end{bmatrix}^T$$

For k =4, order p = 5

$$A = \begin{pmatrix} -\frac{9}{415} & \frac{64}{415} & -\frac{216}{415} & \frac{576}{415} \\ -\frac{576}{3799} & \frac{3375}{3799} & -\frac{8000}{3799} & \frac{9000}{3799} \\ -\frac{1000}{2059} & \frac{5184}{2059} & -\frac{10125}{2059} & \frac{8000}{2059} \\ -\frac{72000}{64171} & \frac{343000}{64171} & -\frac{592704}{64171} & \frac{385875}{64171} \end{pmatrix}, D = \begin{pmatrix} \frac{60}{83} & 0 & 0 & 0 \\ 0 & \frac{4620}{3799} & 0 & 0 \\ 0 & 0 & \frac{3420}{2059} & 0 \\ 0 & 0 & 0 & \frac{133980}{64171} \end{pmatrix} \tag{2.7}$$

$$G = \begin{pmatrix} -\frac{72}{415} & 0 & 0 & 0 \\ 0 & -\frac{1800}{3799} & 0 & 0 \\ 0 & 0 & -\frac{1800}{2059} & 0 \\ 0 & 0 & 0 & -\frac{88200}{64171} \end{pmatrix}$$

$$C_6 = [\frac{24}{2075} \quad \frac{600}{3799} \quad \frac{1800}{2059} \quad \frac{205800}{64171}]^T, E_6 = [\frac{1}{43200} \quad \frac{1}{5184} \quad \frac{1}{1248} \quad \frac{49}{20448}]^T$$

For k =5, order p = 6

$$A = \begin{pmatrix} \frac{144}{12019} & -\frac{1125}{12019} & \frac{400}{12019} & -\frac{9000}{12019} & \frac{16000}{12019} \\ \frac{500}{4669} & -\frac{3456}{4669} & \frac{10125}{4669} & -\frac{16000}{4669} & \frac{13500}{4669} \\ \frac{54000}{128431} & -\frac{343000}{128431} & \frac{889056}{128431} & -\frac{1157625}{128431} & \frac{686000}{128431} \\ \frac{385875}{334699} & -\frac{2304000}{334699} & \frac{5488000}{334699} & -\frac{6322176}{334699} & \frac{3087000}{334699} \\ \frac{5488000}{2134141} & -\frac{31255875}{2134141} & \frac{69984000}{2134141} & -\frac{74088000}{2134141} & \frac{32006016}{2134141} \end{pmatrix}, D = \begin{pmatrix} \frac{8220}{12019} & 0 & 0 & 0 & 0 \\ 0 & \frac{180}{161} & 0 & 0 & 0 \\ 0 & 0 & \frac{192780}{128431} & 0 & 0 \\ 0 & 0 & 0 & \frac{624120}{334699} & 0 \\ 0 & 0 & 0 & 0 & \frac{4735080}{2134141} \end{pmatrix}$$

$$G = \begin{pmatrix} -\frac{1800}{12019} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1800}{4669} & 0 & 0 & 0 \\ 0 & 0 & -\frac{88200}{128431} & 0 & 0 \\ 0 & 0 & 0 & -\frac{352800}{334699} & 0 \\ 0 & 0 & 0 & 0 & -\frac{3175200}{2134141} \end{pmatrix} \tag{2.8}$$

$$C_7 = [\frac{600}{84133} \quad \frac{3600}{32683} \quad \frac{88200}{128431} \quad \frac{940800}{334699} \quad \frac{19051200}{2134141}]^T,$$

$$E_7 = [\frac{5}{19509} \quad \frac{10}{4053} \quad \frac{5}{429} \quad \frac{80}{2049} \quad \frac{180}{1699}]^T$$

For k =6, order p = 7

$$A=\begin{pmatrix} -\frac{100}{13489} & \frac{864}{13489} & -\frac{3375}{13489} & \frac{8000}{13489} & -\frac{13500}{13489} & \frac{21600}{13489} \\ -\frac{21600}{268921} & \frac{171500}{268921} & -\frac{592704}{268921} & \frac{1157625}{268921} & -\frac{1372000}{268921} & \frac{926100}{268921} \\ -\frac{231525}{621139} & \frac{1728000}{621139} & -\frac{5488000}{621139} & \frac{9483264}{621139} & -\frac{9261000}{621139} & \frac{4390400}{621139} \\ -\frac{4390400}{3714811} & \frac{31255875}{3714811} & -\frac{93312000}{3714811} & \frac{148176000}{3714811} & -\frac{128024064}{3714811} & \frac{500009400}{3714811} \\ -\frac{8001504}{2671153} & \frac{54880000}{2671153} & -\frac{156279375}{2671153} & \frac{233280000}{2671153} & -\frac{185220000}{2671153} & \frac{64012032}{2671153} \\ -\frac{1600300800}{244703449} & \frac{10650001824}{244703449} & -\frac{29218112000}{244703449} & \frac{41601569625}{244703449} & -\frac{31049568000}{244703449} & \frac{9861112800}{244703449} \end{pmatrix}$$

$$D=\begin{pmatrix} \frac{1260}{1927} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{280980}{268921} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{859320}{621139} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{6322680}{3714811} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{5370120}{2671153} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{565959240}{244703449} \end{pmatrix}$$

$$G=\begin{pmatrix} -\frac{1800}{13489} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{88200}{268921} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{352800}{621139} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3175200}{3714811} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3175200}{2671153} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{384199200}{244703449} \end{pmatrix} \qquad (2.9)$$

$$C_8=[\frac{450}{94423} \quad \frac{22050}{268921} \quad \frac{352800}{621139} \quad \frac{9525600}{3714811} \quad \frac{23814000}{2671153} \quad \frac{6339286800}{244703449}]^T$$

$$E_8=[\frac{5}{37436} \quad \frac{5}{3428} \quad \frac{5}{647} \quad \frac{135}{4703} \quad \frac{675}{7894} \quad \frac{16335}{74738}]^T$$

For k =7, order p = 8

$$A=\begin{pmatrix} \frac{3600}{726301} & -\frac{34300}{726301} & \frac{148176}{726301} & -\frac{385875}{726301} & \frac{686000}{726301} & -\frac{926100}{726301} & \frac{1234800}{726301} \\ \frac{77175}{1227199} & -\frac{691200}{1227199} & \frac{2744000}{1227199} & -\frac{6322176}{1227199} & \frac{9261000}{1227199} & -\frac{8780800}{1227199} & \frac{4939200}{1227199} \\ \frac{2195200}{6527971} & -\frac{18753525}{6527971} & \frac{69984000}{6527971} & -\frac{148176000}{6527971} & \frac{192036096}{6527971} & -\frac{150028200}{6527971} & \frac{59270400}{6527971} \\ \frac{5334336}{4410583} & -\frac{4390400}{4410583} & \frac{156279375}{4410583} & -\frac{311040000}{4410583} & \frac{370440000}{4410583} & -\frac{256048128}{4410583} & \frac{83349000}{4410583} \\ \frac{1333584000}{388631233} & -\frac{10650001824}{388631233} & \frac{36522640000}{388631233} & -\frac{69335949375}{388631233} & \frac{77623920000}{388631233} & -\frac{49305564000}{388631233} & \frac{14200002432}{388631233} \\ \frac{2465278200}{297202819} & -\frac{19203609600}{297202819} & \frac{63900010944}{297202819} & -\frac{116872448000}{297202819} & \frac{124804708875}{297202819} & -\frac{7451896200}{297202819} & \frac{19722225600}{297202819} \\ \frac{710000121600}{39775926271} & -\frac{5416216205400}{39775926271} & \frac{17579304288000}{39775926271} & -\frac{31197405343104}{39775926271} & \frac{32096096032000}{39775926271} & -\frac{18279729693225}{39775926271} & \frac{4547726726400}{39775926271} \end{pmatrix}$$

$$D=\begin{pmatrix} \frac{457380}{726301} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1212120}{1227199} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{8439480}{6527971} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{6957720}{4410583} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{719638920}{388631233} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{629992440}{297202819} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{94814679960}{39775926271} \end{pmatrix}$$

$$G=\begin{pmatrix} -\frac{88200}{726301} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{352800}{1227199} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3175200}{6527971} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3175200}{4410583} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{384199200}{388631233} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{384199200}{297202819} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{64929664800}{39775926271} \end{pmatrix} \quad (2.10)$$

3.0 The stability of the parallel block SDBDF

When (2.2) 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.

$$M(z) = (I - zD - z^2 G)^{-1}(A + zB) \quad (3.1)$$

***Definition* 3.1**

The stability region of a block method in (2.2) is the region where all amplification factors are less than one in absolute value this will be so when $\rho(M(z)) \le 1$, where $\rho(.)$ is the spectral radius.

***Definition* 3.2**

Method (2.2) is said to be zero stable if $\rho(M(0)) \le 1$, where $\rho(M(0)) = 1$ is simple.

***Definition* 3.3**

Method (2.2) is said to be A-stable if the maximum amplification matrix M(z) is such that $\rho(M(z)) \le 1$, for $z \in C^-$.

***Definition* 3.4**

Method (2.2) is said to be L–stable, if it is A–stable, and such that its amplification factors vanishes at infinity, i.e

$$\lim_{z\to\infty} M(z) = (I - zD - z^2 G)^{-1}(A + zB) = 0 \quad (3.2)$$

Equation (3.2) imply that any *A*–stable method of (2.2) is *L*–stable. The root locus of the stability region is given by the set of points determined by $\rho(M(z)) \le 1$. Below we present root locus plots corresponding to methods (2.5), (2.6), (2.7), (2.8), (2.9) and (2.10).

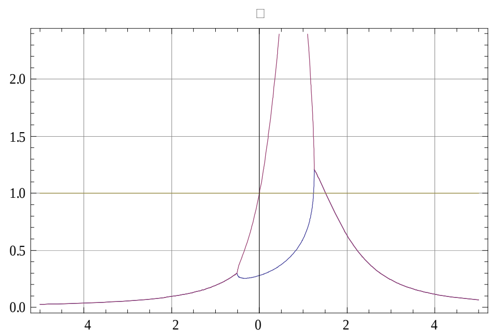

Figure 3.1: Root Locus plot of Method (2.5)

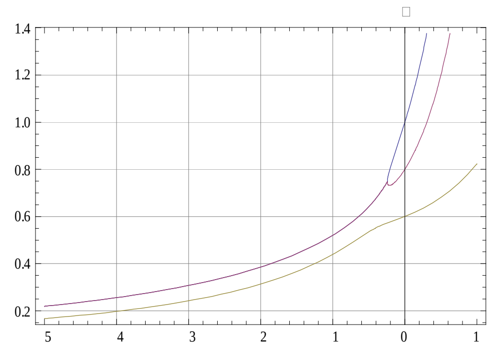

Figure 3.2: Root Locus plot of Method (2.6)

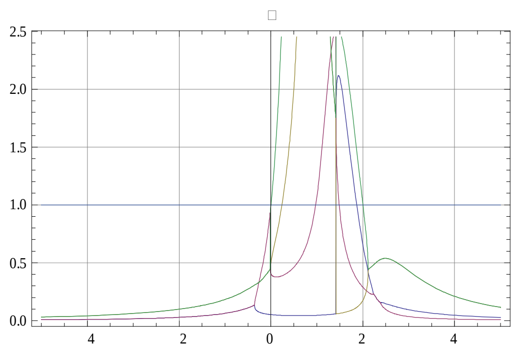

Figure 3.3: Root Locus plot of Method (2.7)

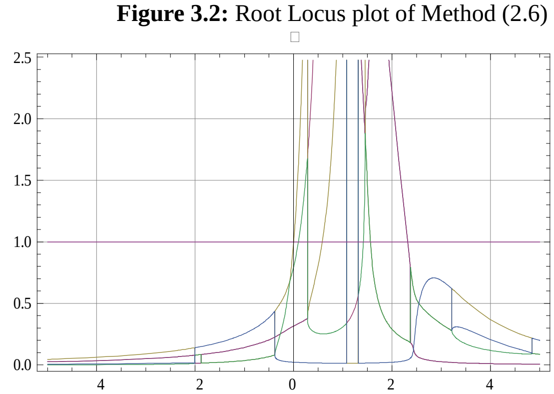

Figure 3.4: Root Locus plot of Method (2.8)

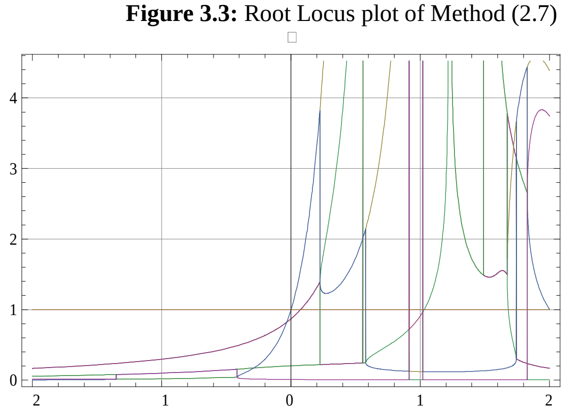

Figure 3.5: Root Locus plot of Method (2.9)

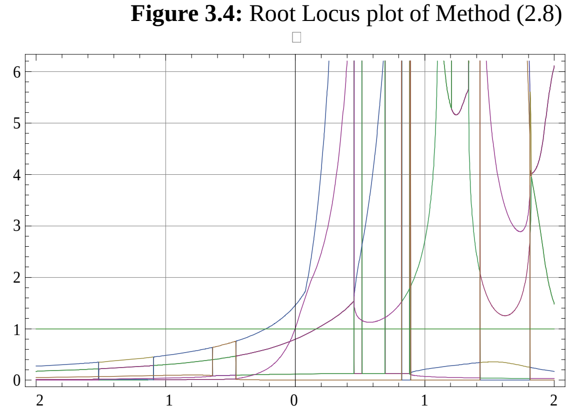

Figure 3.6: Root Locus plot of Method (2.10)

Figures (3.1) – (3.5) clearly show that the amplification factors for block sizes k = 2(1)6 satisfy $|\rho(M(z))| \le 1$ in the entire left region and more so condition (3.2) is satisfied, hence the methods are *L*–stable for block size $k \le 6$. In Figure 3.6 observe that $|\rho(M(z))| > 1$ around the origin; hence SDBDF is zero unstable for block size $k \ge 7$.

4.0 Numerical implementation and conclusion

In order to implement SDBDF, their implicitness are resolve using modified Newton –Raphson's technique suggested by Liniger and Willoughby (See [3]), 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 [4]. Consider the stiff initial value problem given in [3]

$$y' = \begin{bmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{bmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \tag{4.1}$$

We now present the result obtained by integrating (4.1) using SDBDF (2.5) and comparing with the analytical solution.

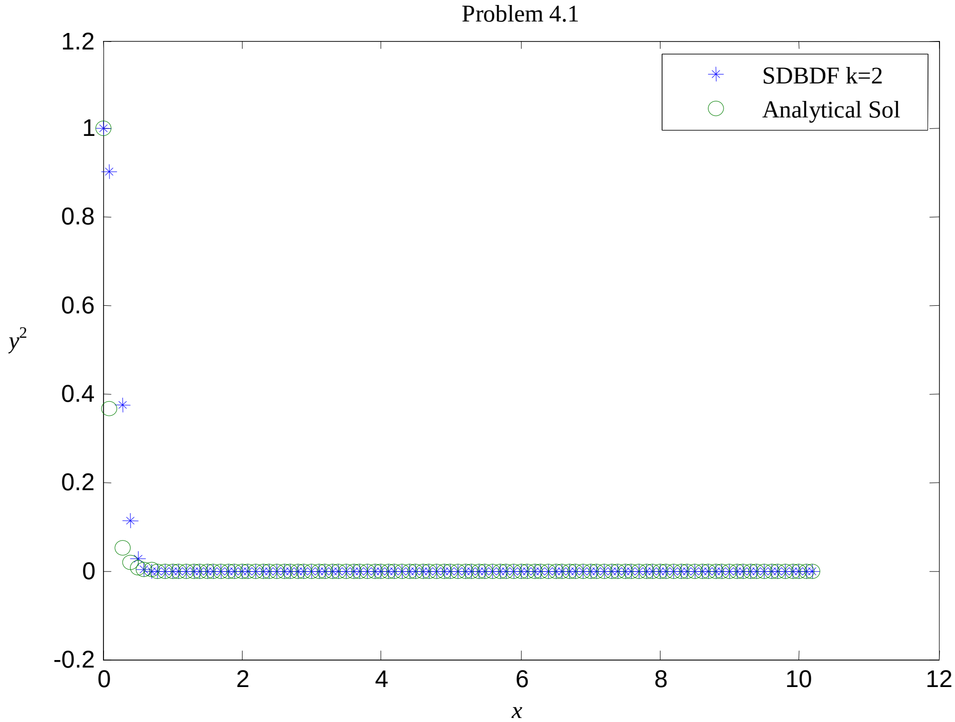

Figure 4.1: Numerical result.

In this paper we considered a class of second derivative parallel block Backward Differentiation Type Formulas (SDBDF). These methods are inherently parallel and are suitable for parallel computers. SDBDF are L-stable for block size $k \leq 6$. Speed up which is computation time gained by using parallel computers are achievable with SDBDF. Hence, SDBDF has an advantage in solving (1.1) faster than methods proposed in [10] and other sequential methods. Normalized error constants of SDBDF are relatively smaller when compared with error constant of methods in [10]. Figure 4.1 presents the graph of the second component of the solution vector of (4.1). In Figure 4.1, the solution component of (4.1) generated by SDBDF mimic the analytic solution.

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