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A (α)-Stable Order Ten Second Derivative Block Multistep Method for Stiff Initial Value Problems

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ABSTRACT : *In this paper, we developed a four step block generalized Adams type second derivative method for the integration of stiff systems in ordinary differential equations. The block method is shown to be A-stable, consistent and zero-stable. Numerical results by the block method reveal that the method is suitable for the solution of stiff initial value problems.*

KEYWORDS: *second derivative, A-stability, block multistep method, stiff system*

I. INTRODUCTION

In this paper we are concerned with the numerical solution of the stiff initial value problem (1) using the second derivative linear multistep.

$$y'(x) = f(x, y(x)),\ \ y(x_0) = y_0 \tag{1}$$

on the finite interval $I = [x_0, x_N]$ where $y : [x_0, x_N] \rightarrow \Re^m$ and $f : [x_0, x_N] \times \Re^m \rightarrow \Re^m$ is continuous and differentiable. The second derivative k-step method takes the following form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\sum_{j=0}^{k} \beta_j f_{n+j} + h^2 \sum_{j=0}^{k} \gamma_j g_{n+j} \tag{2}$$

where α_j, β_j and γ_j are parameters to be determined and $g_{n+j} = f'_{n+j}$. Several authors have considered the numerical solution of (1) by using the usual first derivative methods, for example, [1,2,3] considered the use of the hybrid methods for the solution of (1) in order to overcome the Dahlguist second barrier theorem[4]. Many researchers have studied the second derivative and higher derivative methods because of the existence of A-stable higher multi-derivative formulae as shown by [5, 6,7,8,9,10]. These methods unlike the usual first derivative multistep methods which are not A-stable for orders higher than 2 are A-stable for higher orders. Therefore higher derivative multistep formulae may be suitable for solving stiff equations [11].

In what follows, we shall construct four step block second derivative generalized Adams' type method through interpolation and collocation method of [12]. The continuous formulation of the method evaluated at certain points give rise to four discrete schemes which constitute the second derivative block method for the numerical solution of (1).

This paper is organized as follows: In section 2, the formulation of the block second derivative method is considered. The convergence analysis and the plot of the region of absolute stability of the block method are considered in section 3. Numerical examples are given in section 4 and results obtained are compared with either the exact solutions or the Matlab ode23s in the case where the exact solution is not available and section 5 is about the conclusion of the work.

II. FORMULATION OF THE METHOD

The general form of the four step Generalized Adams'-type second derivative method is of the form

$$y_{n+2} - y_{n+1} = h\sum_{j=0}^{4} \beta_j(x) f_{n+j} + h^2 \sum_{j=0}^{4} \gamma_j(x) g_{n+j} \tag{3}$$

where $\beta_j(x)$ and $\gamma_j(x)$ are the continuous coefficients of the method. We note that y_{n+j} is the numerical approximation to the exact solution $y(x_{n+j})$. $f_{n+j} = f(x_{n+j}, y(x_{n+j})), j = 0,1,2,3,4$ and

$g_{n+j} = f'(x_{n+j}, y(x_{n+j}))$.

The solution of the initial value problem in (1) is assumed to be the polynomial

$$y(x) = \sum_{j=0}^{11} a_j x^j \tag{4}$$

where a_j are unknown coefficients to be determined. To construct the continuous formulation of our method, the conditions imposed in [7] are used as follow;

[1] Equation (4) coincides with the exact solution at the point x_n

[2] The interpolating function (4) satisfies (1) at the points x_{n+j}, $j = 0,1,2,3,4$

[3] The second derivative of (4) coincides with the second derivative of the exact solution at the points x_{n+j}, $j = 0,1,2,3,4$

These conditions result in the following set of 11 equations

$$y(x_{n+1}) = y_{n+1} \tag{5}$$

$$y'(x_{n+j}) = f_{n+j}, \qquad j = 0,1,2,3,4 \tag{6}$$

$$y''(x_{n+j}) = g_{n+j}, \qquad j = 0,1,2,3,4 \tag{7}$$

which is solved to obtained a_j. Substituting the values of a_j into (4) gives the continuous form of the method as

$$y(x) = a_1(x) y_{n+1} + h\sum_{j=0}^{4} \beta_j(x) f_{n+j} + h^2 \sum_{j=0}^{4} \gamma_j(x) g_{n+j} \tag{8}$$

where

$\alpha_1(x) = 1$

$$\beta_0 = \left(\frac{20155\xi^4}{3456h^3} - \frac{42931\xi^5}{8640h^4} + \frac{52025\xi^6}{20736h^5} + \xi - \frac{4745\xi^7}{6048h^6} + \frac{2065\xi^8}{13824h^7} - \frac{1539551}{4354560}h - \frac{247\xi^9}{15552h^8} - \frac{485\xi^3}{144h^2} + \frac{5\xi^{10}}{6912h^9} \right)$$

$$\beta_1 = \left(-\frac{2114\xi^5}{135h^4} + \frac{\xi^{10}}{216h^9} - \frac{89371}{272160}h + \frac{112\xi^4}{9h^3} - \frac{23\xi^9}{243h^8} - \frac{32\xi^3}{9h^2} + \frac{1643\xi^6}{162h^5} - \frac{1423\xi^7}{378h^6} + \frac{701\xi^8}{864h^7} \right)$$

$$\beta_2 = \left(-\frac{57\xi^4}{8h^3} + \frac{3\xi^3}{h^2} - \frac{103}{630}h - \frac{41\xi^6}{12h^5} + \frac{553\xi^5}{80h^4} + \frac{\xi^9}{144h^8} + \frac{51\xi^7}{56h^6} - \frac{\xi^8}{8h^7} \right)$$

$$\beta_3 = -\frac{38341}{272160}h + \frac{1666\xi^5}{135h^4} + \frac{3\text{[illegible]}}{9h^2} - \text{[illegible]}$$

$$\beta_4 = \left(\frac{11879\xi^5}{8640h^4} - \frac{1241\xi^4}{1152h^3} + \frac{203\xi^9}{15552h^8} - \frac{5\xi^{10}}{6912h^9} - \frac{59681}{4354560}h + \frac{53\xi^3}{144h^2} - \frac{1361\xi^8}{13824h^7} - \frac{20089\xi^6}{20736h^5} + \frac{2437\xi^7}{6048h^6} \right)$$

$$\gamma_0 = \left(-\frac{26051}{725760}h^2 + \frac{\xi^2}{2} - \frac{25\xi^3}{18h} + \frac{1045\xi^4}{576h^2} + \frac{2273\xi^6}{3456h^4} + \frac{85\xi^8}{2304h^6} - \frac{199\xi^5}{144h^3} - \frac{25\xi^7}{126h^5} + \frac{\xi^{10}}{5760h^8} - \frac{5\xi^9}{1296h^7} \right)$$

$$\gamma_1 = \left(-\frac{16\xi^3}{3h} + \frac{38\xi^4}{3h^2} + \frac{\xi^{10}}{360h^8} - \frac{19\xi^9}{324h^7} + \frac{31207}{90720}h^2 - \frac{589\xi^5}{45h^3} + \frac{203\xi^6}{27h^4} - \frac{649\xi^7}{252h^5} + \frac{151\xi^8}{288h^6} \right)$$

$$\gamma_2 = \left(\frac{81}{320}h^2 - \frac{781\xi^5}{40h^3} - \frac{6\xi^3}{h} + \frac{403\xi^6}{32h^4} + \frac{33\xi^4}{2h^2} - \frac{19\xi^7}{4h^5} + \frac{\xi^{10}}{160h^8} + \frac{67\xi^8}{64h^6} - \frac{\xi^9}{8h^7} \right)$$

$$\gamma_3 = \left(-\frac{16\xi^3}{9h} + \frac{118\xi^6}{27h^4} - \frac{17\xi^9}{324h^7} - \frac{443\xi^7}{252h^5} + \frac{1243}{18144}h^2 + \frac{\xi^{10}}{360h^8} + \frac{46\xi^4}{9h^2} + \frac{119\xi^8}{288h^6} - \frac{287\xi^5}{45h^3} \right)$$

$$\gamma_4 = \left(\frac{2237}{725760}h^2 + \frac{47\xi^4}{192h^2} + \frac{53\xi^8}{2304h^6} - \frac{113\xi^5}{360h^3} + \frac{\xi^{10}}{5760h^8} - \frac{\xi^3}{12h} - + \frac{769\xi^6}{3456h^4} - \frac{\xi^9}{324h^7} - \frac{47\xi^7}{504h^5} \right) \tag{9}$$

Thus evaluating (8) at $\xi = \{0,2h,3h,4h\}$ we obtain the following block method represented in block matrix finite difference form.

$$AY_m = BY_{m-1} + hCF_m + h^2 D1G_m \tag{10}$$

where

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

C = [redacted]

$$D1 = \begin{bmatrix} -\frac{31207}{90720} & -\frac{81}{320} & -\frac{1243}{18144} & -\frac{2237}{725760} \\ \frac{6887}{90720} & -\frac{47}{320} & -\frac{1721}{90720} & -\frac{103}{145152} \\ \frac{269}{2835} & -\frac{269}{2835} & 0 & -\frac{11}{5670} \\ \frac{183}{1120} & \frac{81}{320} & \frac{279}{1120} & -\frac{339}{8960} \end{bmatrix}$$

The 4-dimensional vector Y_m, Y_{m-1}, F_m and G_m have collocation points specified as

$$Y_m = [y_{n+1}, y_{n+2}, y_{n+3}, y_{n+4}]^T$$

$$Y_{m-1} = [y_{n-3}, y_{n-2}, y_{n-1}, y_n]^T$$

$$F_m = [f_{n+1}, f_{n+2}, f_{n+3}, f_{n+4}]^T$$

$$G_m = [g_{n+1}, g_{n+2}, g_{n+3}, g_{n+4}]^T$$

III. ANALYSIS OF THE METHOD

We present here the analysis of the block method in (10). Convergence which is an important property required of all good linear multistep methods shall be investigated for the block method and the region of absolute stability plotted.

Local truncation error : In the spirit of [13,14], the local truncation error associated with the block method (10) is the linear difference operator

$$L[Y(x):h] = \sum_{j=0}^{k} \left\{ \alpha_j Y(x+jh) - hY'\beta_j(x+jh) - h^2 Y''\gamma_j(x+jh) \right\} \quad (11)$$

We assume that $Y(x)$ is sufficiently differentiable, and so the terms of (11) can be expanded as Taylor series about x to give the expression

$$L[Y(x):h] = C_0 Z(x) + C_1 hZ'(x) + \ldots + C_q h^q Z^{(q)}(x) + \ldots \quad (12)$$

where

$$C_0 = \sum_{j=0}^{k} \alpha_j$$

$$C_1 = \sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k} \beta_j$$

$$C_2 = \tfrac{1}{2}\sum_{j=1}^{k} j^2\alpha_j - \sum_{j=1}^{k} j\beta_j - \sum_{j=0}^{k} \gamma_j$$

$$\vdots$$

$$C_q = \tfrac{1}{q!}\sum_{j=1}^{k} j^q\alpha_j - \tfrac{1}{(q-1)!}\sum_{j=1}^{k} j^{q-1}\beta_j - \tfrac{1}{(q-2)!}\sum_{j=1}^{k} j^{q-2}\gamma_j, q = 3,4,..$$

The block method (10) is said to be of order p if $\overline{C}_0 = \overline{C}_1 = \ldots = \overline{C}_p = \overline{0}, \quad \overline{C}_{p+1} \neq \overline{0}.$

$\overline{C}_{p+1}$ is called the error constant and the local truncation of the method is given as

$$\bar{t}_{n+k} = \overline{C}_{p+1} h^{(p+1)} y^{(p+1)} x_n + O(h^{(p+1)}). \quad (13)$$

The block method (10) has order and error constant of $p = (10,10,10,10)^T$ and $C_{11} = \left(\frac{551}{314344800}, \frac{89}{314344800}, \frac{89}{157172400}, \frac{1}{431200}\right)^T$ respectively. Since the block method (10) is of order $p = 10 \geq 1$, it is consistent [15].

Zero Stability of the Block method

The block method (10) is said to be zero stable provided the roots $R_j, \ j = 1,...,k$ of the first characteristic polynomial $\rho(R)$ specified by

$$\rho(R) = \det\left[\sum_{i=0}^{k} A^{(i)} R^{k-i}\right] = 0 \tag{14}$$

satisfies $\left|R_j\right| \leq 1, \ j = 1,...,k.$ and for those roots with $\left|R_j\right| = 1,$ the multiplicity does not exceed 2. Applying the usual test equations

$$y' = \lambda y\,, \qquad y'' = \lambda^2 y$$

to the block method (10) with $z = \lambda y$ and solving the characteristic equation

$$det\left(r\left(A - Cz - D1z^2\right) - B\right) = 0$$

for r at $z = 0$ yields the following roots {0, 0, 0, 1}. The block method is therefore zero stable since the absolute value of each of the roots is less than or equal to 1.

3.3 Convergence

The block method is convergent since it is both consistent and zero stable [15].

3.4 Region of Absolute Stability of new method

Solving characteristic equation $det\left(r\left(A - Cz - D1z^2\right) - B\right) = 0$ for r, we obtain the stability function as

$$R(z) = \frac{-3(3578238z^6 - 8007630z^5 + 280279845z^4 + 1454723035z^3 + 4627627200z^2 + 626330880z + 3857868000)}{25128z^8 + 8722148z^7 - 149522390z^6 + 985089480z^5 - 378826396z^4 + 1115687473z^3 - 2076308640z^2 + 2314720800z - 1157360400} \tag{15}$$

The region of absolute stability of the block method is obtained by substituting $det\left(r\left(A - Cz - D1z^2\right) - B\right)$ and its derivative into a matlab code.

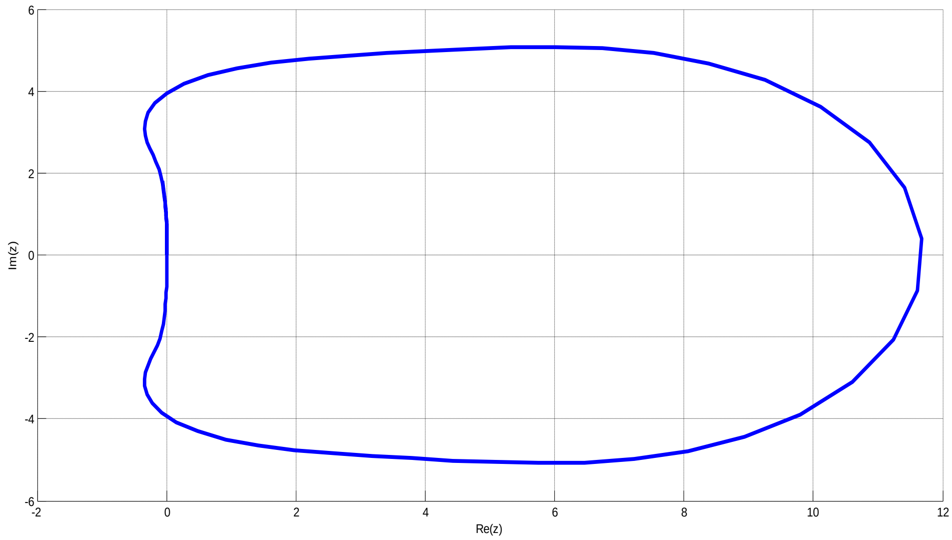

Figure1: Region of Absolute Stability of the Block method (10)

IV. NUMERICAL EXPERIMENTS

In this section, we present some numerical results to compare the performance of our new method with the analytic solution and with the Matlab ode solver ode23s where the analyticsolution is not available.

Example 1: Chemistry Problem Considered by [16]

$$\begin{aligned} y_1' &= -0.013y_1 - 1000y_1y_3, & y_1(0) &= 1, \\ y_2' &= -2500y_2y_3, & y_2(0) &= 1, \\ y_3' &= -0.013y_1 - 1000y_1y_3 - 2500y_2y_3, & y_3(0) &= 0. \end{aligned}$$

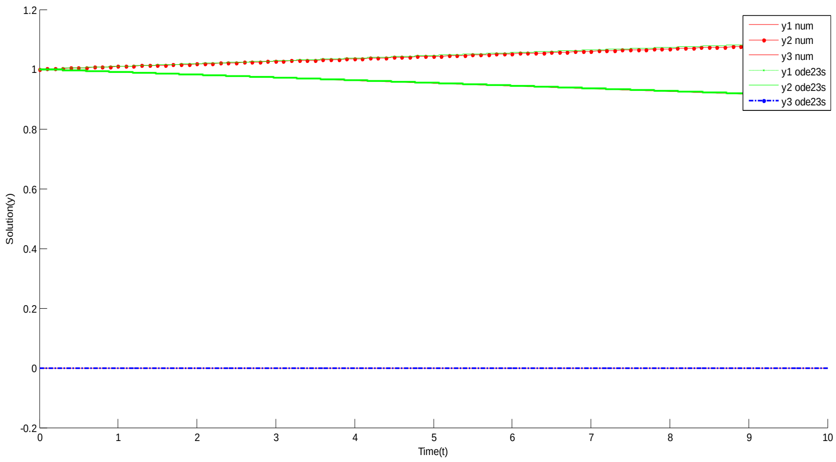

Figure 2: Solution curve for example 1 using the new block method (10)

Example 2: We consider another linear problem which is particularly referred to by some eminent authors [17, 18] as a troublesome problem for some existing methods. This is because some of the eigenvalues lying close to the imaginary axis, a case where some stiff integrators are known to be inefficient.

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \\ y_3'(x) \\ y_4'(x) \\ y_5'(x) \\ y_6'(x) \end{bmatrix} = \begin{bmatrix} -10 & 100 & 0 & 0 & 0 & 0 \\ -100 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.1 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \\ y_4(x) \\ y_5(x) \\ y_6(x) \end{bmatrix}, \quad \begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \\ y_4(0) \\ y_5(0) \\ y_6(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

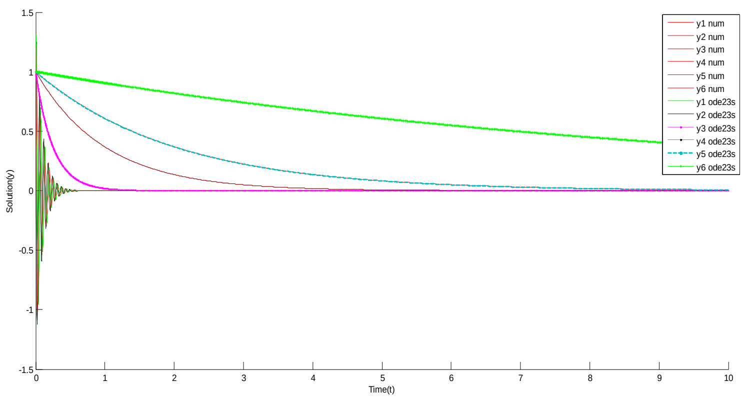

Figure 2: Solution curve for example 2 using the new block method (10)

Example 3: The third problem is a well-known classical system. It is a mildly stiff problem composed of two first order equations,

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \end{bmatrix} = \begin{bmatrix} 998 & 1998 \\ -999 & -1999 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix}, \quad \begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix},$$

and the exact solution is given by the sum of two decaying exponential components,

$$\begin{cases} y_1(x) = 4e^{-x} - 3e^{-1000x} \\ y_2(x) = -2e^{-x} + 3e^{-1000x} \end{cases}$$

The stiffness ratio is 1:1000. We solve the problem in the interval [0, 10].

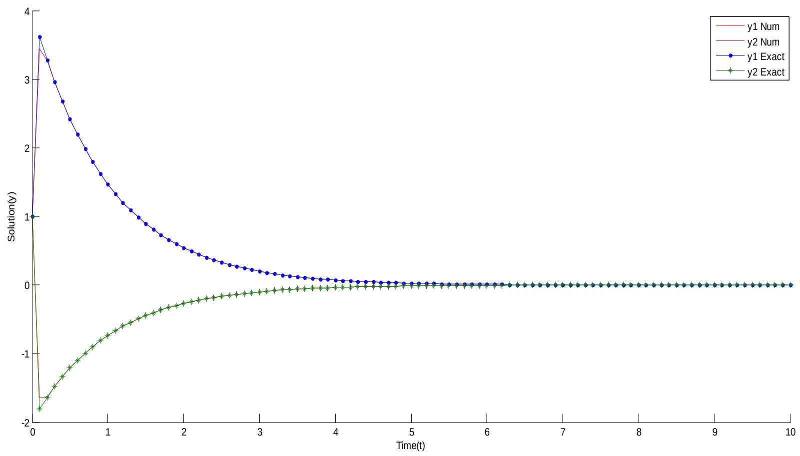

Figure3: Solution curve for problem 3 using the new block method (10)

Table1: Absolute Errors for Problem 3 using the new block method (10)

x	Error y1	Error y2
20	7.64E-13	3.93E-13
40	1.95E-13	9.89E-14
60	5.55E-14	2.79E-14
80	6.44E-15	3.25E-15
100	1.29E-15	6.47E-16

Example 4

$$y'_1 = -8y_1 + 7y_2$$
$$y'_2 = 42y_1 - 43y_2$$
$$y_1(0) = 1, \quad y_2(0) = 8, \qquad 0 \le x \le 10, \;\; h = 0.1$$
$$y_1(x) = 2e^{-x} - e^{-50x}, \;\; y_2(x) = -2e^{-x} + 6e^{-50x}$$

Table2: Absolute Errors for Problem 4 using the new block method (10**)**

x	Error y1	Error y2
20	1.17E-15	1.17E-15
40	2.29E-16	2.29E-16
60	3.30E-17	3.30E-17
80	6.07E-18	6.07E-18
100	9.35E-19	9.35E-19

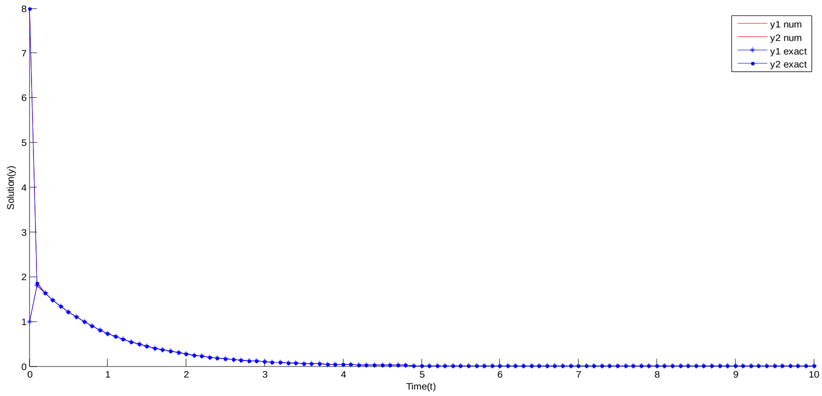

Figure4: Solution curve for problem 4 using the new block method (10)

V. CONCLUSION

The construction of a block three step multistep method for the solution of stiff initial value problems is considered. Some numerical properties of the block method were investigated and the method is shown to be of uniform order p = 10, consistent and zero-stable and with good region of absolute stability. We have also demonstrated the accuracy of our block method on some linear and non linear stiff system. The numerical results show that our method competes favourably well with the Matlab ode solver ode23s.

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