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SIMPSON'S $\frac{3}{8}$-TYPE BLOCK METHOD FOR STIFF SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT. In this paper, a self-starting second derivative multistep block method which uses the logic behind the Simpson's 3/8 rule for quadrature is derived using collocation and interpolation techniques to obtain the approximate solutions of stiff differential equations. The main method and two additional methods are assembled into a block matrix equation which is applied to provide the solutions of stiff IVPs on non-overlapping intervals.. The method is shown to be A-Stable, effective and reliable for stiff systems of ordinary differential equations. The order of the method is discussed and its accuracy is tested and established numerically.

Keywords and phrases: Simpson's $\frac{3}{8}$ rule, Block Method, Second Derivative, A-Stability, Stiff Systems
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1. INTRODUCTION

Numerical solutions for ordinary differential equations (ODEs) are very important in scientific computation, as they are widely used for solutions of real world problems. In many applications modeled by systems of ordinary differential equations, these systems exhibit a behaviour known as stiffness. Stiff systems are considered difficult because explicit numerical methods designed for non-stiff problems are used with very small step sizes or do not converge at all. The knowledge of stiffness, occurring in differential equations came as a result of some pioneering works done by the two chemists, Curtiss and Hirschfelder [8]. In 1979, Shampine and Gear [23] in their text, they expounded the characteristics of numerical methods used for solving problems with stiffness and discussed the different realistic goals when solving stiff problems which involves methods with strong stability properties for solving stiff systems.

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Consider the differential equations of the form

$$y' = f(t, y),\ y(t_0) = y_0\ ,\ x \in [t_0, T_n]$$

where f satisfies the Lipschitz condition as given in Henrici [15]). The k-step LMM is conventionally written as

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

Which has $2k+1$ unknown α's and β's and therefore can be of order $2k$, where k is is the step number, however, according to Dahlquist[9], the order of (2) cannot exceed $k+1$ (k is odd) or $k+2$ (k is even) for the method to be stable. Several authors such as Lambert [18], Gear[12], Gragg and Stetter[13], Butcher[5], Akinfenwa et-al[1] proposed modified forms of (2) known as hybrid methods which were shown to overcome the Dahlquist barrier theorem. Several other methods have been proposed for efficiently solving (1) (see Keiper and Gear [17], Enright([11], [10]), Hairer and Wanner[14], Cash[6] and Brugnano and Trigiante[4]).Recently Sahi et.al.[21] presented the Simpson's type second derivative A-stable block method of order six which uses the logic of Simpson' $\frac{1}{3}$ rule, and adapted to cope with the integration of stiff systems in ordinary differential equations.

In the spirit of Sahi et.al.[21], the logic behind the Simpson's $\frac{3}{8}$-rule for quadrature is used to construct a second derivative multistep block method, using the techniques of interpolation and collocation. A main discrete method and two additional methods are obtained from the same continuous scheme and assembled into a block matrix equation which is applied to provide the solutions for (1). The advantage of a block method is that in each application, the solution is approximated at more than one point. The number of points depends on the structure of the block method. Therefore, applying these methods can give faster solutions to the problem which can be managed to produce a desired accuracy.

This paper is organized as follows: In section 2, the derivation of the block method is considered. The convergence analysis and the plot of region of absolute stability of the block method are discussed in section 3. Numerical examples are given in section 4 to show the efficiency of the derived method. Section 5 of the paper gives the conclusion of the work.

2. Derivation of the method

The Simpson's $\frac{3}{8}$-type block second derivative method is of the form

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

where k=1,2,3 and β_j, γ_j, for each case are coefficients to be determined. We proceed by assuming that the exact solution $y(t)$ is locally represented in the range $[t_0, t_0 + 3h]$ by the continuous solution $Y(t)$ of the form

$$Y(t) = \sum_{j=0}^{8}\zeta_j\phi_j(t) \tag{3}$$

where ζ_j are unknown coefficients to be determined and $\phi_j(t)$ are polynomial basis functions. The method is then constructed with $\phi_j(t) = t^j, j = 0, \ldots, 8$ by imposing the following conditions
(i) The interpolating function (4) coincides with the analytical solution $y(t)$ at the mesh point t_n
(ii) Equation (4) satisfies (1) at mesh points t_{n+j},$j = 0, 1, 2, 3$.
(iii) The second derivative of (4) coincides with the second derivative of the analytical solution at mesh points $t_{n+j}, j = 0, 1, 2, 3$.
The imposed conditions lead to a system of nine equations of the form

$$Y(t) = y_n \tag{4}$$

$$Y'(t) = f_{n+i},\ i = 0, 1, 2, 3 \tag{5}$$

$$Y''(t) = g_{n+i},\ i = 0, 1, 2, 3 \tag{6}$$

It should be noted that equation (5),(6)and (7) lead to a system of equations which must be solved to obtain the coefficients $\zeta_j, j = 0, \ldots, 8$ which are substituted into (4) and after some algebraic computation, our continuous representation yields the form

$$Y(t) = \alpha_j(t)y_n + h\sum_{j=0}^{3}\beta_j(t)f_{n+j} + h^2\sum_{j=0}^{3}\gamma_j(t)g_{n+j} \tag{7}$$

where $\alpha_j(t)$, $\beta_j(t)$ and $\gamma_j(t)$ are continuous coefficients. The equation (8) is then used to obtain the main method by evaluating (8) at point $t = t_{n+3}$, and the additional methods at points $t = t_{n+2}$ and $t = t_{n+1}$. The combination these methods yields the block method:

$$\left.\begin{array}{l} y_{n+3} = y_n + \frac{3h}{224}[31f_n + 81f_{n+1} + 81f_{n+2} + 31f_{n+3}] \\ \quad + \frac{3h^2}{1120}[19g_n - 27g_{n+1} + 27g_{n+2} - 19g_{n+3}] \\ y_{n+2} = y_n + h[\frac{223}{567}f_n + \frac{20}{21}f_{n+1} + \frac{13}{21}f_{n+2} + \frac{20}{567}f_{n+3}] \\ \quad +h^2[\frac{43}{945}g_n - \frac{16}{105}g_{n+1} - \frac{19}{105}g_{n+2} - \frac{8}{945}g_{n+3}] \\ .y_{n+1} = y_n + h[\frac{6893}{18144}f_n + \frac{313}{672}f_{n+1} + \frac{89}{672}f_{n+2} + \frac{397}{18144}f_{n+3}] \\ \quad +h^2[\frac{1283}{30240}g_n - \frac{851}{3360}g_{n+1} - \frac{269}{3360}g_{n+2} - \frac{163}{30240}g_{n+3}] \end{array}\right\} \quad (8)$$

From our analysis the integrators (9) are found to be of order p= $(8, 8, 8)^T$ with error constants
$C_{p+1}{=}C_9 = (\frac{9}{313600}, \frac{13}{793800}, \frac{313}{25401600})^T$

3. Stability Analysis

In what follows, (9) can be rearranged and rewritten as a matrix finite difference equation to assume the block form

$$A^{(1)}Y_\omega = A^{(0)}Y_{\omega-1} + h[B^{(1)}F_\omega + B^{(0)}F_{\omega-1} + h^2[C^{(1)}G_\omega + C^{(0)}G_{\omega-1}] \quad (9)$$

where
$$\begin{aligned} Y_\omega &= (y_{n+1}, y_{n+2}, y_{n+3})^T, \\ Y_{\omega-1} &= (y_{n-2}, y_{n-1}, y_n)^T, \\ F_\omega &= (f_{n+1}, f_{n+2}, f_{n+3})^T, \\ F_{\omega-1} &= (f_{n-2}, f_{n-1}, f_n)^T, \\ G_\omega &= (g_{n+1}, g_{n+2}, g_{n+3})^T, \\ G_{\omega-1} &= (g_{n-2}, g_{n-1}, g_n)^T, \end{aligned}$$

for $\omega = 0, \ldots$ and $n = 0, 3, \ldots, N-3$ and the matrices $A^{(1)}$, $A^{(0)}$, $B^{(1)}$,$B^{(0)}$ $C^{(1)}$ and $C^{(0)}$are three dimensional matrices whose entries are given by the coefficients of (9) defined as follow:

$$A^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$A^{(0)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

$$B^{(1)} = \begin{pmatrix} \frac{313}{672} & \frac{89}{672} & \frac{397}{18144} \\ \frac{20}{21} & \frac{13}{21} & \frac{20}{567} \\ \frac{243}{224} & \frac{243}{224} & \frac{93}{224} \end{pmatrix}$$

$$B^{(0)} = \begin{pmatrix} 0 & 0 & \frac{6893}{18144} \\ 0 & 0 & \frac{223}{567} \\ 0 & 0 & \frac{93}{224} \end{pmatrix}$$

$$C^{(1)} = \begin{pmatrix} \frac{-851}{3360} & \frac{-269}{3360} & \frac{-163}{30240} \\ \frac{-16}{105} & \frac{-19}{105} & \frac{-8}{945} \\ \frac{-81}{1120} & \frac{81}{1120} & \frac{-57}{1120} \end{pmatrix}$$

$$C^{(0)} = \begin{pmatrix} 0 & 0 & \frac{1283}{30240} \\ 0 & 0 & \frac{43}{945} \\ 0 & 0 & \frac{57}{1120} \end{pmatrix}$$

Zero Stability: It is worth noting that zero-stability is concerned with the stability of the difference system in the limit as h tends to zero. Thus, as $h \to 0$, the method (10) tends to the difference system

$$A^{(1)}Y_\omega - A^{(0)}Y_{\omega-1} = 0$$

whose first characteristic polynomial $\rho(R)$ is given by

$$\rho(R) = \det(RA^{(1)} - A^{(0)}) = R^2(R-1) \tag{10}$$

Following Fatunla[**?**], the block method (10) is zero-stable, since from (11), $\rho(R) = 0$ satisfies $|R_j| \leq 1$, $j = 1, 2, 3$, and for those roots with $|R_j| = 1$, the multiplicity does not exceed 1.

Consistency: The block method (10) is consistent as it has order $p > 1$. According to Henrici[15] the method is convergent, since $convergence = zerostability + consistency$.

Linear stability: The linear stability property of (10) is determined by applying it to the test equation $y' = \lambda y,\ \lambda < 0$ to yield

$$Y_\omega = \sigma(z)Y_{\omega-1}\ ,\ z = \lambda h, \tag{11}$$

where the matrix $\sigma(z)$ is given by

$$\sigma(z) = -(A^{(1)} - zB^{(1)} - z^2C^{(1)})^{-1}(A^{(0)} + zB^{(0)} + z^2C^{(0)})$$

From (12) we obtain the stability function $R(z) : \mathbb{C} \to \mathbb{C}$ which is a rational function with real coefficients given by

$$R(z) = \frac{3z^6 + 33z^5 + 193z^4 + 720z^3 + 1740z^2 + 2520z + 1680}{3z^6 - 33z^5 + 193z^4 - 720z^3 + 1740z^2 - 2520z + 1680} \tag{12}$$

The stability domain of the method (or region of absolute stability) S is defined as

$$S = [z \ \epsilon\ \mathbb{C} : R(z) \leq 1] \tag{13}$$

Specifically, when the left-half complex plane is contained in S, the method is said to be A-stable. In Figure 1, The plot in shaded portion represents the stability region which corresponds to the stability function $R(z)$.

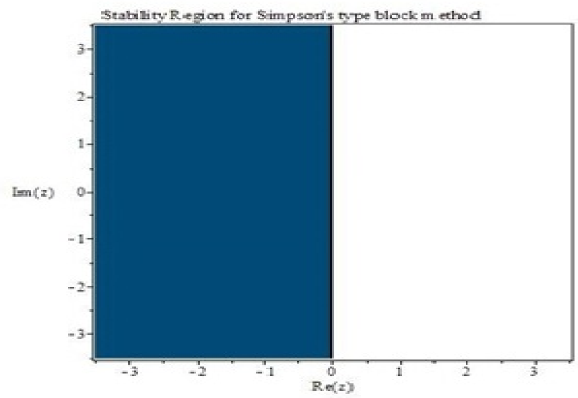

Fig. 1. Stability Region

Clearly, from Figure 1, it is obvious that our method is A- stable since stability function is contained in the left half complex plane.

4. IMPLEMENTATION

The implementation of the above block methods is summarized as follows: On the partition

$I_N : \{a = t_0 < t_1 < \ldots < t_{N-1} < t_N = b\}$, $n = 0, 1, 2, \ldots, N-1$

Step 1. Choose N for $k = 3$, $h = \frac{b-a}{N}$ the number of blocks $\pi = \frac{N}{3}$ using (10) $n = 0, \omega = 1$ the values $(y_1, y_2, y_3)^T$ are generated simultaneously over the subinterval $[t_0, t_3]$ as y_0 are known from the IVP (1).

Step 2. for $n = 3, \omega = 2$, $(y_3 \ldots, y_6)^T$ are obtained over the subinterval $[t_3, t_6]$ since y_3 is known from the first block

Step 3. The process is continued for $n = 2k, \ldots, N-k$ and $\omega = 3, \ldots, \pi$ to obtain approximate solutions to (1) on sub-intervals $[t_0, t_k], \ldots, [t_{N-k}, t_N]$ N is a positive integer and n the grid index.

5. NUMERICAL EXAMPLES

In this section, we discuss the implementation of the Simpson's-type block method on some standard stiff systems of ordinary differential equations. In order to show the accuracy of the method, five numerical examples, together with the results are presented in this section. All numerical computations were executed using our written code on Maple 17. For linear problem we use the Gaussian elimination to solve the resulting k x k matrix in each block. While for non- linear problems the code uses the Newton iteration.

Example 5.1

Our first example is the strongly stiff system on the range $0 \leq t \leq 1$

$$y_1' = -500000y_1 + 499999.5y_2,\ y_1(0) = 0$$
$$y_2' = 499999.5y_1 - 500000.5y_2,\ y_2(0) = 2$$

Its exact solution is given by the sum of two decaying exponentials components

$$y_1 = -e^{-\lambda_1 t} + e^{-\lambda_2 t}$$
$$y_2 = e^{-\lambda_1 t} + e^{-\lambda_2 t}$$

$\lambda_1 = 10^{-6}$, $\lambda_2 = -1$

This problem with stiffness ratio $1 : 10^6$ has been solved by Tahmasbi [24] using the modification of the power series method. The results in [24] are represented in Table 1 and compared with the results obtained from the newly derived method. From Table 1, it is obvious that the derived method performs better even for a bigger step size. for the solution .

Table 1. The absolute error for Example 5.1

t	Error in modified [24] power series method h=0.00001 y_1 y_2	Error in New Method h=0.0001 y_1 y_2
0.2	6.20×10^{-14}	3.93×10^{-25}
	6.20×10^{-14}	3.93×10^{-25}
0.4	1.02×10^{-13}	6.57×10^{-25}
	1.02×10^{-13}	6.57×10^{-25}
0.6	6.05×10^{-14}	8.00×10^{-25}
	6.05×10^{-14}	8.00×10^{-25}
0.8	4.48×10^{-14}	8.72×10^{-25}
	4.48×10^{-14}	8.72×10^{-25}
1.0	4.41×10^{-14}	8.90×10^{-25}
	4.41×10^{-14}	8.90×10^{-25}

Example 5.2

Consider the Stiffly nonlinear problem which was proposed by Kaps [16] in the range $0 \leq t \leq 10$

$$y_1' = (\epsilon^{-1} + 2)y_1 + \epsilon^{-1}y_2,\ y_1(0) = 1$$
$$y_2' = y_1 - y_2 - y_2^2,\ y_2(0) = 1$$

the smaller ϵ is, the more serious the stiffness of the system. Its exact solution is given by $y_1 = y_2^2$, $y_2 = e^{-t}$ We compare the new method with that of $M(8, r8)$ in Chartier [7] and $BBDF_8$ in Akinfenwa et.al.[2] taking $\epsilon = 10^{-8}$ for the correct digit $\Delta = -\log_{10}\left(\frac{||y_i(T) - y_{n,i}||_\infty}{||y_{n,i}||_\infty}\right)$ at the end of the interval for various values of h as shown in
It can be seen that for this example the New method show superiority over the methods compared.

Table 2. A comparison of methods for the number of correct digits Δ using $\epsilon = 10^{-8}$ for Example 5.2

method	$h = 1/4$	$h = 1/8$	$h = 1/16$	$h = 1/32$	$h = 1/64$	$h = 1/128$
$M(8, r8)$	4.66	5.67	6.26	8.47	10.8 3	15.63
$BBDF_8$	5.80	7.93	10.21	12.52	12.87	12.58
$NewMethod$	8.52	10.94	13.35	15.76	18.16	19.97

Example 5.3 Consider the nonlinear system of differential equation in the range $0 \leq t \leq 10$

$$y_1' = \mu y_1 + y_2^2,\ y_1(0) = -\frac{1}{(\mu + 2)}$$
$$y_2' = -y_2\ y_2(0) = 1$$

Where $\mu = 10000$. the exact solution is $y_1 = -\frac{e^{-2t}}{(\mu+2)}$, $y_2 = e^{-t}$ We compare the new method with that of Second derivative multistep methods (SDMM) in Mehdizadeh et.al. [20] as shown in Table 3. The new method is superior to that in Mehdizadeh et.al. [20].

Table 3: A comparison of methods for Example 5.3

t	Error in Mehdizadeh et.al. [20] h=0.0001 y_1 y_2	Error in New Method h=0.1 y_1 y_2
3	2.478147×10^{-11}	2.029806×10^{-19}
	2.471093×10^{-6}	1.437435×10^{-14}
5	3.450271×10^{-14}	1.204486×10^{-20}
	2.304573×10^{-8}	3.214575×10^{-15}
10	3.456372×10^{-18}	1.114598×10^{-20}
	3.150734×10^{-11}	4.375846×10^{-17}

Example 5.4

Consider the non-linear stiff problem:

$$y_1' = -0.04y_1 + 10^4 y_2 y_3 \ y_1(0) = 1$$

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

$$y_3' = 3 \times 10^7 y_2^2 \ y_3(0) = 0$$

This is a chemical problem suggested by H.H. Robertson [22] in (1966), which is used to test stiff integrators. The problem is solved with the newly derived method in the range $0 \le t \le 40$ and the results for $t = 0.4, \ 40$ with step size h=0.001 are presented in Table 4 below.

Table 4: A comparison of methods for Example 5.4

t	Y	SDMM [20]	HSDMM [19]	New Method
0.4	y_1	$9.851721113863 \times 10^{-1}$	$9.851721113863 \times 10^{-1}$	$9.851721113792 \times 10^{-1}$
	y_2	$3.386395378909 \times 10^{-5}$	$3.386395378909 \times 10^{-5}$	$3.386395377787 \times 10^{-5}$
	y_3	$1.479402218548 \times 10^{-2}$	$1.479402218548 \times 10^{-2}$	$1.479402225356 \times 10^{-2}$
40	y_1	$7.158270687189 \times 10^{-1}$	$7.158270687189 \times 10^{-1}$	$7.158270687143 \times 10^{-1}$
	y_2	$9.185534764567 \times 10^{-6}$	$9.185534764567 \times 10^{-6}$	$9.185534764362 \times 10^{-6}$
	y_3	$2.841637457463 \times 10^{-1}$	$2.841637457463 \times 10^{-1}$	$2.841637457508 \times 10^{-1}$

Example 5.5

next we solve the standard stiff problem which arose from a chemistry problem. The problem is solved with the newly derived method in the range $0 \le t \le 2$ and the results for $t = 2$ with step size h=0.0001 are presented in Table 5 below. Consider the non-linear stiff problem:

$$y_1' = -0.013y_1 - 1000y_1y_2 - 2500y_1y_3 \ y_1(0) = 0$$

$$y_2' = -0.013y_1 - 1000y_1y_2 \ y_2(0) = 1$$

$$y_3' = -2500 y_1 y_3 \ y_3(0) = 1$$

Table 5: A comparison of methods for Example 5.5

t	Y	Exact	New Method
2	y_1	$-0.3616933169289 \times 10^{-5}$	$-0.3616933169289 \times 10^{-5}$
	y_2	0.9815029948230	0.9815029948230
	y_3	1.018493388244	1.018493388244

Example 5.6

As our last example, we consider a well known classical system {see [25]} in the range $0 \leq t \leq 100$

$$y_1' = 998y_1 + 1998y_2, \ y_1(0) = 1$$
$$y_2' = -999y_1 - 1999y_2, \ y_2(0) = 1$$

Its exact solution is given by the sum of two decaying exponentials components

$$y_1 = 4e^{-t} - 3e^{-1000t}$$
$$y_2 = -2e^{-t} + 3e^{-1000t}$$

The stiffness ratio is 1 : 1000. In Table 6, we present result for methods in [25] and compare with the newly derived method at the points $T = 5, 40, 70 and 100$ using the step length $h = 0.1$. The Simpson 3/8 type of order eight performs better than methods 3.2 and 3.4 of order eight and eleven respectively. order eight

Table 6: Absolute errors $= |y_i(T) - y_i|$ at various point of T for Example 5.6

T	Method 3.2 in [25] $p = 8$ $Erry_1$	$Erry_2$	Method 3.4 in [25] $p = 11$ $Erry_1$	$Erry_2$	$New Method$ $p = 8$ $Erry_1$	$Erry_2$
5	1.96×10^{-2}	9.80×10^{-1}	1.58×10^{-2}	7.92×10^{-3}	8.56×10^{-3}	8.56×10^{-3}
40	3.81×10^{-7}	1.91×10^{-7}	1.02×10^{-7}	5.11×10^{-8}	6.06×10^{-14}	6.06×10^{-14}
70	8.91×10^{-12}	4.45×10^{-12}	9.16×10^{-13}	4.58×10^{-13}	1.70×10^{-23}	1.70×10^{-23}
100	2.08×10^{-18}	1.04×10^{-18}	6.67×10^{-18}	3.33×10^{-18}	4.76×10^{-33}	4.76×10^{-33}

5. CONCLUDING REMARKS

A self-starting Simpson's 3/8 type second derivative block method , for solving stiff ordinary differential equation has been proposed. The good stability and consistency property show that the method is effective and reliable for numerical solution of stiff problems. The accuracy of the method has been tested on both linear and nonlinear stiff problems, signifying that the derived method is highly efficient and competitive with other existing stiff solvers.

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