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Improved family of block methods for special second order initial value problems [I.V.Ps].

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Abstract

In this paper, efforts are directed towards generating a 2-block 3-point numerical method for solving the special second order initial value problems of the form $Y'' = F(X,Y)$, $Y(0) = Y_O$, $Y'(0) = Y_{OO}$, where Y' is the total derivative of Y with respect to X. The scheme so developed, is an extension of Aladeselu, V.A (2006)[1], in which a 2-block 2-point scheme was developed.. The scheme is of orders 8/9, zero-stable and convergent. It is thus possible, with this scheme, to assign computational tasks at 3 points within the block to three different processors working simultaneously.

Key words: block; special second order i.v..p; numerical methods, PECE.

1.0 Introduction.

Traditional computers are built on the Von Nuemann model of computation which is on the concept of a single central processing unit (C.P.U), which has access to a linear array of fixed-sized cells, called memory.

Due to the fact that modern problems are characterized by computational complexities that are either difficult to solve or take unduly long time to solve by the Von Nuemann model of computation, on one hand , and the recent advances in speed and memory capacity of supercomputers, on the other hand, it has become necessary to modify existing algorithms or develop new algorithms to cope with the numerical solutions of the special second order initial value problem of the form

$$Y'' = F(X,Y),\ Y(0) = Y_0,\ Y'(0) = Y_{00} \qquad (1.1).$$

Problems of the form (1.1), where Y' is absent in F, are of interest because they often occur in satellite tracking/warning systems; celestial mechanics; mass action kinetics, solar systems, molecular biology and spatial discretization of Hyperbolic partial differential equations or spatial discretization of infinite dimensional systems. However, the theoretical solutions of these equations are usually highly oscillatory and so restricts, very severely, the mesh-size, h, of the conventional Linear Multistep Method (LMM)

$$\sum\alpha_j\, y_{n+j} = h^2\sum\beta_j\, f_{n+j},\ j = 0(1)k \qquad (1.2)$$

where y_n is the numerical approximation to the theoretical solution $y(x_n)$ at $x = x_n$ and $f_n = f(x_n, y_n) = y'_n$.

In this paper, we propose a 2-block 3-point numerical integrators of orders 8/9, by extending the ideas in Aladeselu (2006)[1]. The resultant numerical integrators possess the following desirable properties:

(a) Zero-stability i.e stability at the origin;
(b) Cheap and reliable error estimates;
(c) Facility to generate solutions at 3 points simultaneously.
(d) Ability to generate higher order schemes with relatively smaller step-sizes than the equivalent traditional LMM (1.2)

2.0 Development of Scheme

The r-point k-step block method for the equation (1.1), Aladeselu(2006)[1], was represented by the matrix difference equation

$$0 = \Sigma A^{(i)} y_{m-i} + h^2 \Sigma B^{(i)} f_{m-i},\ i = 0(1)k \qquad (2.1)$$

where, 0, $A^{(i)}$, $B^{(i)}$, are r by r real matrices, $A^{(0)}$ is an identity matrix of order r and y_{m-i} , f_{m-i}, are r-vectors such that

$$y_m = (y_{n+1}, y_{n+2}, y_{n+3}, \ldots, y_{n+r-1}, y_{n+r},)$$
$$f_m = (f_{n+1}, f_{n+2}, f_{n+3}, \ldots, f_{n+r-1}, f_{n+r},) \qquad (2.2)$$

In this paper, our focus is on $r = 3$, $k = 2$ and so $n = mr = 3m$, while

$$A^{(i)} = \begin{bmatrix} a_{11}^{(i)} & a_{12}^{(i)} & a_{13}^{(i)} \\ a_{21}^{(i)} & a_{21}^{(i)} & a_{23}^{(i)} \\ a_{31}^{(i)} & a_{32}^{(i)} & a_{33}^{(i)} \end{bmatrix},\ B^{(i)} = \begin{bmatrix} b_{11}^{(i)} & b_{12}^{(i)} & b_{13}^{(i)} \\ b_{21}^{(i)} & b_{21}^{(i)} & b_{23}^{(i)} \\ b_{31}^{(i)} & b_{32}^{(i)} & b_{33}^{(i)} \end{bmatrix},\ i = 0(1)2 \qquad (2.3)$$

***Assumption* 2.1**

The scheme (2.1) is normalized for easy analysis and consistency of scheme.

Let $z_m = [y(x_{n+1}),\ y(x_{n+2}),\ y(x_{n+3})]^T$ be the theoretical solution of equation (1.1) and let it be sufficiently differentiable. If Taylor's series expansion is applied to $z(x)$, $z(x + jh)$ and $z^{//}(x + jh)$ and then inserted in the linear difference operator

$$L[z(x), h] = \Sigma [\alpha_j z(x + jh) - h^2 \beta_j z^{//}(x + jh)],\ j=0(1)\infty \qquad (2.4),$$

it follows that

$$L[z(x), h] = \Sigma c_v h^v z^{(v)}(x) + 0(h^{q+1}),\ v = 0(1)q \qquad (2.5)$$

where the c_v's , which are independent of $z(x)$, are called error constants given by the relation

$$C_v = (1/v!)\ [\Sigma j^v \alpha_j - v(v-1)\Sigma j^{v-2}\beta_j],\ j = 0(1)k,\ (k = 2, \text{ in this case}) \qquad (2.6)$$

***Definition* 2.2**

The order P of the difference operator L in (2.4) and consequently of the LMM (1.2) is a unique integer which is defined by the relations

$$C_v = 0 \text{ for all } v = 0(1)P + 1 \text{ and } C_{p+2} \neq 0. \qquad (2.7)$$

Now $y_m = (y_{n+1}, y_{n+2}, y_{n+3})^T = (y_{3m+1}, y_{3m+2}, y_{3m+3})^T$, since in this case, $n = mr = 3m \Rightarrow y_{m-1} = (y_{3(m-1)+1}, y_{3(m-1)+2}, y_{3(m-1)+3})^T = (y_{3m-2}, y_{3m-1}, y_{3m})^T = (y_{n-2}, y_{n-1}, y_n)^T$. Similarly, it can be shown that $y_{m-2} = (y_{n-5}, y_{n-4}, y_{n-3})^T$; $f_m = (f_{n+1}, f_{n+2}, f_{n+1})^T$; $f_{m-1} = (f_{n-2}, f_{n-1}, f_n)^T$; $f_{m-2} = (f_{n-5}, f_{n-4}, f_{n-3})^T$.

Using these last six results in equation (2.1) gives

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} y_{n-1} \\ y_{n-2} \\ y_{n-3} \end{bmatrix} = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ a_{21}^{(1)} & a_{21}^{(1)} & a_{23}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} \end{bmatrix}\begin{bmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix} + \begin{bmatrix} a_{11}^{(2)} & a_{12}^{(2)} & a_{13}^{(2)} \\ a_{21}^{(2)} & a_{21}^{(2)} & a_{23}^{(2)} \\ a_{31}^{(2)} & a_{32}^{(2)} & a_{33}^{(2)} \end{bmatrix}\begin{bmatrix} y_{n-5} \\ y_{n-4} \\ y_{n-3} \end{bmatrix}$$

$$+ h^2 \begin{bmatrix} b_{11}^{(0)} & b_{12}^{(0)} & b_{13}^{(0)} \\ b_{21}^{(0)} & b_{21}^{(0)} & b_{23}^{(0)} \\ b_{31}^{(0)} & b_{32}^{(0)} & b_{33}^{(0)} \end{bmatrix}\begin{bmatrix} f_{n-1} \\ f_{n-2} \\ f_{n-3} \end{bmatrix} + \begin{bmatrix} b_{11}^{(1)} & b_{12}^{(1)} & b_{13}^{(1)} \\ b_{21}^{(1)} & b_{21}^{(1)} & b_{23}^{(1)} \\ b_{31}^{(1)} & b_{32}^{(1)} & b_{33}^{(1)} \end{bmatrix}\begin{bmatrix} f_{n-2} \\ f_{n-1} \\ f_n \end{bmatrix} + \begin{bmatrix} b_{11}^{(2)} & b_{12}^{(2)} & b_{13}^{(2)} \\ b_{21}^{(2)} & b_{21}^{(2)} & b_{23}^{(2)} \\ b_{31}^{(2)} & b_{32}^{(2)} & b_{33}^{(2)} \end{bmatrix}\begin{bmatrix} f_{n-5} \\ f_{n-4} \\ f_{n-3} \end{bmatrix}$$

which componentwisely can be written as

$$y_{n+q} = \sum_{t=1}^{t=2}\sum_{s=1}^{s=3} a_{qs}(t) y_{n+s-3t} + h^2 \sum_{t=0}^{t=2}\sum_{s=1}^{s=3} b_{qs}(t) f_{n+s-3t},\quad q = 1(1)3 \qquad (2.8)$$

Case q = 1

$$y_{n+1} = a_{11}^{(1)}y_{n-2} + a_{12}^{(1)}y_{n-1} + a_{13}^{(1)}y_n + a_{11}^{(2)}y_{n-5} + a_{12}^{(2)}y_{n-4}^{(2)} + a_{13}^{(2)}y_{n-3}$$
$$+ h^2[b_{11}^{(0)}f_{n+1} + b_{12}^{(0)}f_{n+2} + b_{13}^{(0)}f_{n+3} + b_{11}^{(1)}f_{n-2} + b_{12}^{(1)}f_{n-1} + b_{13}^{(1)}f_n + b_{11}^{(2)}f_{n-5} + b_{12}^{(1)}f_{n-4} + b_{13}^{(2)}f_{n-3}].$$

Matching with the LMM

$$\sum \alpha_j y_{n-j+r} = h^2 \sum \beta_j f_{n-j+r},\ j = 0(1)m,\ \text{m} = r(k+1) - 1\ (= 8 = p, \text{ in this case}) \qquad (2.9)$$

it follows that

$\alpha_0 = 0 = \alpha_1$, $\alpha_2 = 1$, $\alpha_3 = -a_{13}^{(1)}$, $\alpha_4 = -a_{12}^{(1)}$, $\alpha_5 = -a_{11}^{(1)}$, $\alpha_6 = a_{13}^{(2)}$, $\alpha_7 = -a_{12}^{(2)}$, $\alpha_8 = -a_{11}^{(2)}$

$\beta_0 = b_{13}^{(0)}$, $\beta_1 = b_{12}^{(0)}$, $\beta_2 = b_{11}^{(0)}$, $\beta_3 = b_{13}^{(1)}$, $\beta_4 = b_{12}^{(1)}$, $\beta_5 = b_{11}^{(1)}$, $\beta_6 = b_{13}^{(2)}$, $\beta_7 = b_{12}^{(2)}$, $\beta_8 = b_{11}^{(2)}$

$$\Rightarrow \quad a_{13}^{(1)} + a_{12}^{(1)} + a_{11}^{(1)} + a_{13}^{(2)} + a_{12}^{(2)} + a_{11}^{(2)} = 1$$
$$3a_{13}^{(1)} + 4a_{12}^{(1)} + 5a_{11}^{(1)} + 6a_{13}^{(2)} + 7a_{12}^{(2)} + 8a_{11}^{(2)} = 2$$

Set $a_{11}^{(1)} = 0 = a_{11}^{(2)}$, and $a_{12}^{(1)} = 0 = a_{12}^{(2)}$ in the last two equations to obtain $a_{13}^{((1)} = 4/3$, $a_{13}^{(2)} = -1/3$. By setting $c_j = 0$, for $j = 2(1)9$ and $b_{13}^{(0)} = \alpha$, a free parameter, the following 8 relations were obtained

$$b_{12}^{(0)} + b_{11}^{(0)} + b_{13}^{(1)} + b_{12}^{(1)} + b_{11}^{(1)} + b_{13}^{(2)} + b_{12}^{(2)} + b_{11}^{(2)} = 2 - \alpha$$
$$b_{12}^{(0)} + 2b_{11}^{(0)} + 3b_{13}^{(1)} + 4b_{12}^{(1)} + 5b_{11}^{(1)} + 6b_{13}^{(2)} + 7b_{12}^{(2)} + 8b_{11}^{(2)} = 22/3$$
$$b_{12}^{(0)} + 4b_{11}^{(0)} + 9b_{13}^{(1)} + 16b_{12}^{(1)} + 25b_{11}^{(1)} + 36b_{13}^{(2)} + 49b_{12}^{(2)} + 64b_{11}^{(2)} = 85/3$$
$$b_{12}^{(0)} + 8b_{11}^{(0)} + 27b_{13}^{(1)} + 64b_{12}^{(1)} + 125b_{11}^{(1)} + 216b_{13}^{(2)} + 343b_{12}^{(2)} + 512b_{11}^{(2)} = 115$$
$$b_{12}^{(0)} + 16b_{11}^{(0)} + 81b_{13}^{(1)} + 256b_{12}^{(1)} + 625b_{11}^{(1)} + 1296b_{13}^{(2)} + 2401b_{12}^{(2)} + 4096b_{11}^{(2)} = 7322/15$$
$$b_{12}^{(0)} + 32b_{11}^{(0)} + 243b_{13}^{(1)} + 1024b_{12}^{(1)} + 3125b_{11}^{(1)} + 7776b_{13}^{(2)} + 16807b_{12}^{(2)} + 32768b_{11}^{(2)} = 6466/3$$
$$b_{12}^{(0)} + 64b_{11}^{(0)} + 729b_{13}^{(1)} + 4096b_{12}^{(1)} + 15625b_{11}^{(1)} + 46656b_{13}^{(2)} + 117649b_{12}^{(2)} + 262144b_{11}^{(2)} = 137845/14$$
$$b_{12}^{(0)} + 128b_{11}^{(0)} + 2187b_{13}^{(1)} + 16384b_{12}^{(1)} + 78125b_{11}^{(1)} + 279936b_{13}^{(2)} + 823543b_{12}^{(2)}$$
$$+ 2097152b_{11}^{(2)} = 833375/18$$

$\Rightarrow \quad b_{11}^{(0)} = 80/1(7!) + 28\alpha$, $b_{12}^{(0)} = 7791/18(7!) - 8\alpha$;

$b_{11}^{(1)} = 32594/18(7!) - 56\alpha$,

$b_{12}^{(1)} = 58030/18(7!) + 70\alpha$;

$b_{13}^{(1)} = 81300/18(7!) - 56\alpha$,

$b_{11}^{(2)} = -31/18(7!) + \alpha$,

$b_{12}^{(2)} = 184/18(7!) - 8\alpha$;

$b_{13}^{(2)} = 1563/18(7!) + 28\alpha$

Case q = 2

By setting $a_{21}^{(1)} = 0 = a_{21}^{(2)}$, $a_{22}^{(1)} = 0 = a_{22}^{(2)}$ and $b_{23}^{(0)} = \beta$, a free parameter, the following results were obtained , employing the same technique as above:

$a_{23}^{(1)} = 5/3$; $a_{23}^{(2)} = -2/3$

$\Rightarrow \quad b_{22}^{(0)} = 11359/36(7!) - 8\beta$,

$\Rightarrow \quad b_{21}^{(0)} = 49538/9(7!) + 28\beta$;

$b_{23}^{(1)} = 102103/12(7!) - 56\beta$,

$b_{22}^{(1)} = 137975/18(7!) + 70\beta$,

$b_{21}^{(1)} = 95945/36(7!) - 56\beta$,

$b_{23}^{(2)} = 1913/3(7!) + 28\beta$;

$b_{22}^{(2)} = -3917/36(7!) - 8\beta$,

$b_{21}^{(2)} = 223/18(7!) + \beta$

Case q = 3

By setting $a_{31}^{(1)} = 0 = a_{31}^{(2)}$, $a_{32}^{(1)} = 0 = a_{32}^{(2)}$ and $b_{33}^{(0)} = \gamma$, a free parameter, the following results were obtained , employing the same technique as above:

$a_{33}^{(1)} = 2$, $a_{33}^{(2)} = -1$

$\Rightarrow \quad b_{32}^{(0)} = 32022/4(7!) - 8\gamma$,

$b_{31}^{(0)} = 1647/4(7!) + 28\gamma$,

$b_{33}^{(1)} = 32967/(7!) - 56\gamma$,

$b_{32}^{(1)} = -51651/4(7!) + 70\gamma$.

$b_{31}^{(1)}$ = 92934/4(7!) - 56γ,
$b_{33}^{(2)}$ = -34263/4(7!) + 28γ,
$b_{32}^{(2)}$ = 2538/(7!) - 8γ; $b_{31}^{(2)}$ = -1269/4(7!) + γ

Thus the resultant 2-block 3-point scheme is given by the relation

$$y_m = \begin{bmatrix} 0 & 0 & \frac{4}{3} \\ 0 & 0 & \frac{5}{3} \\ 0 & 0 & 2 \end{bmatrix} y_{m-1} + \begin{bmatrix} 0 & 0 & -\frac{1}{3} \\ 0 & 0 & -\frac{2}{3} \\ 0 & 0 & -1 \end{bmatrix} y_{m-2} + h^2 \left[\begin{bmatrix} 8045/18(7!)+28\alpha & 7791/18(7!)-8\alpha & \alpha \\ 99076/18(7!)+28\beta & 11359/36(7!)-8\beta & \beta \\ 1647/14(7!)+28\gamma & 32022/4(7!)-8\gamma & \gamma \end{bmatrix} fm \right.$$

$$+ \begin{bmatrix} 32594/18(7!)-56\alpha & 58039/18(7!)+70\alpha & 81300/18(7!)-56\alpha \\ 95945/36(7!)-56\beta & 275950/36(7!)+70\beta & 306309/36(7!)-56\beta \\ 92934/4(7!)-56\gamma & -516512/4(7!)+70\gamma & 32967/7-56\gamma \end{bmatrix} f_{m-1} + \begin{bmatrix} -31/18(7!)+\alpha \\ 446/36(7!)+\beta \\ -1269/4(7!)+\gamma \end{bmatrix} \text{ with}$$

$$\left. \begin{matrix} 184/18(7!)-8\alpha & 1563/18(7!)+28\alpha \\ -3917/18(36!)-8\beta & 22956/36(7!)+28\beta \\ 10152/4(7!)-8\gamma & -34263/4(7!)+28\gamma \end{matrix} \right] f_{m-2} \qquad (2.10)$$

error constant C_{10} = (3.511676036 × 10^{-4} - α, -2.00307264 × 10^{-3} - β, -3.68678819 -γ$)^T$ and of order 8 , which is also evident from (2.9) in which r = 3, k = 2.

The scheme (2.10) will be of order 9 if C_{10} = (0, 0, 0$)^T$ in which case α = 0.0003511676036, β = -0.00200307264, and γ = -3.68678819.

3.0 Zero-stability test for scheme 2.10

The first characteristic polynomial of the block method (2.10) is given by the relation ρ(R) = $|\Sigma A^{(i)}R^{(2-i)}|$ = 0, i = 0(1)2

=>$R^2(R^2(R^2 - 2R + 1)) = 0$ => R=0(4 times), 1(twice). Thus scheme is zero-stable. Hence, by Henrici(1962)[4], scheme 2.10 is convergent as it is zero-stable and of order greater than 1.

3.1 Explicit form

Suppose the scheme of interest is explicit. Then the coefficients of matrix $B(0)$ will each be zero and as such , employing the same procedure to obtain scheme (2.10), relation (2.8) takes the form

$$y_m^{(0)} = \begin{bmatrix} 0 & 0 & \frac{4}{3} \\ 0 & 0 & \frac{5}{3} \\ 0 & 0 & 2 \end{bmatrix} y_{m-1} + \begin{bmatrix} 0 & 0 & -\frac{1}{3} \\ 0 & 0 & -\frac{2}{3} \\ 0 & 0 & -1 \end{bmatrix} y_{m-2} + h^2 \left[\begin{bmatrix} 1324 & -356 & 986 \\ 20840 & -13855 & 6880 \\ 124578 & -82782 & 29079 \end{bmatrix} f_{m-1} \right.$$

$$\left. \begin{bmatrix} -52 & 314 & -776 \\ -1055 & 6280 & -15490 \\ -6966 & 40743 & -98172 \end{bmatrix} f_{m-2} \right] \qquad (2.11)$$

Scheme (2.11) is of order 6 and has error constant C_8, where C_8 = (0.069080688, 1.53034061, 11.20044643$)^T$

The scheme (2.11) could be adopted as a predictor for scheme (2.10), which could it self be used as a corrector. We adopted this approach and applied them to the scalar test equation

$$\mathbf{y}'' = -100y \; ; \; y(0) = 1 \text{ and } y'(0) = 10 .$$

The following tables were obtained at $x = \pi$.

Table 3.1 (Output comparison)

H	Theoretical Solution = 1.000001430511475		Point
	Predictor	**Corrector**	
0.001	1.000021815299988 1.000052094459534 1.000092506408691	1.000022649765015 1.000052094459534 1.000092506408691	First Second Third
0.0025	1.000126838684082 1.000314593315125 1.000565052032471	1.000132322311401 1.000314593315125 1.000565052032471	First Second Third
0.005	1.000501751899719 1.001252174377441 1.002252578735352	1.000523924827576 1.001252174377441 1.002252578735352	First Second Third

Table 3.2 (Error comparison)

H	Errors in		Point
	Predictor	**Corrector**	
0.001	-2.038478851318359D-05 -5.066394805908203D-05 -9.107589721679688D-05	-2.121925354003906D-05 -5.066394805908203D-05 -9.107589721679688D-05	First Second Third
0.0025	-1.254081726074219D-04 -3.131628036499023D-04 -5.636215209960938D-04	-1.308917999267578D-04 - 3.131628036499023D-04 -5.636215209960938D-04	First Second Third
0.005	-5.003213882446289D-04 -1.250743865966797D-03 -2.251148223876953D-03	-5.2449431610107742D-04 -1.250743865966797D-03 -2.251148223876953D-03	First Second Third

4.0 Conclusion

In this paper, we developed 2-block 3-point numerical integrators of orders 8/9. The resultant numerical integrators possess the following desirable properties:

(a) Zero-stability i.e stability at the origin;
(b) Cheap and reliable error estimates;
(c) Facility to generate solutions at 3 points simultaneously.
(d) Ability to generate higher order schemes with relatively smaller step-sizes than the equivalent traditional LMM (1.2)
(e) It is Convergent scheme

In addition, the new scheme compares favourably with the theoretical solution. Recall that it is a desirable property for a numerical solution to behave similar to the theoretical solution to a problem at all times. Secondly, it is more accurate than Aladeselu, V.A.[1].

The normal approach to implement these schemes is to adopt the $P(EC)^{\delta}E$ mode for some $\delta > 1$ (ideally, $\delta \leq 3$). After every integration step (or attempt), we exploit the error at the immediate past integration step to select a new step size given by the relation

$$h_{new} = 0.9 * (\text{tolerance}/\text{error}_n)^{(1/p)} * h_{old} ,$$

where p is order of scheme, h_{old} is the step size adopted in the last attempt, either a successful or a failed step and h_{new}, is the step size to adopt for the next integration step, tolerance is the specified error tolerance while error_n , is the computed error in the last integration step.

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