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A 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 2-point numerical method for solving the special second order initial value problems of the form $Y^{//} = F(X, Y)$, $Y(0) = Y_O$, $Y^{/}(0) = Y_{OO}$ .. The scheme so developed, is in the same line of thought as Shampine and Watts (1969, 1972) [9]; Chu and Hamltion (1987) [2]; Fatunla (1991)[3]. The scheme is of orders 5/6, zero-stable and convergent. It is thus possible, with this scheme, to assign computational tasks at 2 points within the block to two different processors working simultaneously.

1.0 Introduction

Traditional computers are built on the Von Neumann 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 Neumann 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 initial value problem of the form

$$Y'' = F(X,Y),\ Y(0) = Y_0,\ Y(0) = Y_\infty\ Y^{//} = F(X,Y), \quad (1.1).$$

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 meshsize, *h*, of the conventional Linear Multistep Method (LMM)

$$\sum \alpha_J y_{n+j} = h^2 \sum \beta_j f_{n+j}\ \Sigma \alpha_j y_{n+j} \quad (1.2)$$

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

Several numerical integrators to solve problems characterized by equation (1.1) have been developed. Prominent among these are Gear (1967,1971); Brown (1974); Enright (1974); Chawla (1981); Fatunla (1978,1980,1981, 1988, 1991, 1993); Lambert and Watson (1975); Sharp (1979), who proposed an R-stable Runge-Kutta-Nystrom mehods.

In this paper, we propose 2-block 2-point numerical integrators of orders 5/6, by extending the ideas in Fatunla (1991, 1993). 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 2 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), Fatunla (1991) [3], was represented by the matrix difference equation

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

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

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

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

$$A^{(i)} = \begin{pmatrix} a_{11}^{(i)} & a_{12}^{(i)} \\ a_{21}^{(i)} & a_{22}^{(i)} \end{pmatrix}, \quad B^{(i)} = \begin{pmatrix} b_{11}^{(i)} & b_{12}^{(i)} \\ b_{21}^{(i)} & b_{22}^{(i)} \end{pmatrix}, \; i = 0,1,2 \qquad (2.3)$$

***Assumption* 2.1**

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

Let $z_m = [y(x_{n+1}), y(x_{n+2})]^T$ 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 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

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

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 2.1

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

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

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

Using these last six results in equation (2.1) gives

$$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} y_{a+1} \\ y_{a+2} \end{pmatrix} = \begin{pmatrix} a_{11}^{(1)} & a_{12}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} \end{pmatrix}\begin{pmatrix} y_{n-11} \\ y_n \end{pmatrix} + \begin{pmatrix} a_{11}^{(2)} & a_{12}^{2} \\ a_{21}^{(2)} & a_{22}^{(2)} \end{pmatrix}\begin{pmatrix} y_{n-3} \\ y_{n-2} \end{pmatrix} + h^2\left(\begin{pmatrix} b_{11}^{(0)} & b_{12}^{(0)} \\ b_{22}^{(0)} & b_{22}^{(0)} \end{pmatrix}\begin{pmatrix} f_{n+1} \\ f_{n+2} \end{pmatrix}\begin{pmatrix} b_{11}^{((1)} & b_{12}^{(1)} \\ b_{21}^{(1)} & b_{22}^{(1)} \end{pmatrix}\begin{pmatrix} f_{n-1} \\ f_n \end{pmatrix}\right.$$

$$\left. + \begin{pmatrix} b_{11}^{(1)} & b_{12}^{(1)} \\ b_{21}^{(1)} & b_{22}^{(1)} \end{pmatrix}\begin{pmatrix} f_{n-1} \\ f_n \end{pmatrix} + \begin{pmatrix} b_{11}^{(2)} & b_{12}^{(2)} \\ b_{21}^{(2)} & b_{22}^{(2)} \end{pmatrix}\begin{pmatrix} f_{n+1} \\ f_{n+2} \end{pmatrix}\right)$$

which componentwisely can be written as

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

Case q = 1

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

Matching with the LMM

$$\Sigma \alpha_j y_{n-j+r} = h^2 \Sigma \beta_j f_{n-j+r} , j = 0(1)m', \; m' = r(k + 1) - 1 \; (= 5 = p, \text{in this case}) \ldots \qquad (2.9)$$

It follows that $\alpha_0 = 0$, $\alpha_1 = 1$, $\alpha_2 = - a_{12}^{(1)}$ $\alpha_3 = - a_{11}^{(1)}$, $\alpha_4 = - a_{12}^{(2)}$, $\alpha_5 = - a_{11}^{(2)}$

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

=> $a_{12}^{(1)} + a_{11}^{(1)} + a_{12}^{(2)} + a_{11}^{(2)} = 1$

$2a_{12}^{(1)} + 3a_{11}^{(1)} + 4a_{12}^{(2)} + 5a_{11}^{(2)} = 1$

$b_{12}^{(0)} + b_{11}^{(0)} + b_{12}^{(1)} + b_{11}^{(1)} + b_{12}^{(2)} + b_{11}^{(2)} = 1 - 4a_{12}^{(1)} - 9a_{11}^{(1)} - 6a_{12}^{(2)} - 25a_{11}^{(2)}$

$b_{11}^{(0)} + 2b_{12}^{(1)} + 3b_{11}^{(1)} + 4b_{12}^{(2)} + 5b_{11}^{(2)} = 1 - 8a_{12}^{(1)} - 27a_{11}^{(1)} - 64a_{12}^{(2)} - 1\,25a_{11}^{(2)}$

$b_{11}^{(0)} + 4b_{12}^{(1)} + 9b_{11}^{(1)} + 16b_{12}^{(2)} + 25b_{11}^{(2)} = 1 - 16a_{12}^{(1)} - 81a_{11}^{(1)} - 256a_{12}^{(2)} - 625a_{11}^{(2)}$

$b_{11}^{(0)} + 8b_{12}^{(1)} + 27b_{11}^{(1)} + 64b_{12}^{(2)} + 12\,5b_{11}^{(2)} = 1 - 32a_{12}^{(1)} - 243a_{11}^{(1)} - 1024a_{12}^{(2)} - 31\,25a_{11}^{(2)}$

$b_{11}^{(0)} + 16b_{12}^{(1)} + 81b_{11}^{(1)} + 256b_{12}^{(2)} + 625b_{11}^{(2)} = 1 - 64a_{12}^{(1)} - 729a_{11}^{(1)} - 4096a_{12}^{(2)} - 15625a_{11}^{(2)}$

Setting $a_{11}^{(1)} = 0 = a_{11}^{(2)}$ and $b_{12}^{(0)} = \alpha$, a free parameter, it was found that $a_{12}^{(1)} = 1.5$, $a_{12}^{(2)} = -0.5$ and the b's are given as follows:

$b_{11}^{(0)} = 37/480 - 5\alpha$; $b_{12}^{(1)} = 9/10 = + \alpha$; $b_{11}^{(1)} = 37/80 - 10\alpha$

$b_{12}^{(2)} = 1/15 + 5\alpha$; $b_{11}^{(2)} = -1/160 - \alpha$

Case *q* = 2

$\alpha_0 = 1,\ \alpha_1 = 0,\ \alpha_2 = -a_{22}^{(1)}\ \ \alpha_3 = -a_{21}^{(1)},\ \alpha_4 = -a_{22}^{(2)},\ \alpha_5 = -a_{21}^{(2)}$

$\beta_0 = b_{22}^{(0)},\ \beta_1 = b_{21}^{(0)},\ \beta_2 = b_{22}^{(1)},\ \beta_3 = b_{21}^{(1)},\ \beta_4 = b_{22}^{(2)},\ \beta_5 = b_{21}^{(2)}$

Similar but appropriate set of equations were obtained for the second componentas per above. By setting $a_{21}^{(1)} = 0 = a_{21}^{(2)}$ and $b_{12}^{(0)} = \beta$, a free parameter, the following results were obtained $a_{22}^{(1)} = 2$, $a_{22}^{(2)} = -1$ and the *b*'s are given as follows:

$b_{21}^{(0)} = 21/15 - 5\beta$; $b_{22}^{(1)} = 16/15 + 10\beta$; $b_{21}^{(1)} = 26/15 - 10\beta$

$b_{22}^{(2)} = -4/15 + 5\beta$; $b_{21}^{(2)} = 1/15 - \beta$

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

$$y_m = \begin{pmatrix} 0 & 1\cdot 5 \\ 0 & 2 \end{pmatrix} y_{m-1} + \begin{pmatrix} 0 & -1\cdot 5 \\ 0 & -1 \end{pmatrix} y_{m-2} + h^2 \left(\begin{pmatrix} 37/480 - 5\alpha & \alpha \\ 21/15 - 5\beta & \beta \end{pmatrix} f_m + \begin{pmatrix} 37/80 - 10\alpha & 9/10 + 10\alpha \\ 26/15 - 10\beta & 16/15 + 10\beta \end{pmatrix} f_{m-1} + \begin{pmatrix} -1/160 - \alpha & 1/15 + 5\alpha \\ 1/15 - \beta & -4/15 + 5\chi \end{pmatrix} f_m \right) \qquad (2.10)$$

with error constant $C_7 = (0.00416666667 - \alpha,\ -0.0672222222 - \beta)^T$. Thus it is of order 5, which is also evident from (2.9) in which *r* = 2, *k* = 2

The scheme (2.10) will be of order 6 if $C_7 = (0, 0)^T$ in which case $\alpha = 0.00416666667$ and $\beta = -0.0672222222$ while the scheme takes the form

$$y_m = \begin{pmatrix} 0 & 1\cdot 5 \\ 0 & 2 \end{pmatrix} y_{m-1} + \begin{pmatrix} 0 & -1\cdot 5 \\ 0 & -1 \end{pmatrix} y_{m-2} + h^2 \left(\begin{pmatrix} 0\cdot 05625 & 0\cdot 0041\check{7} \\ 1\cdot 80278 & -0\cdot 06722 \end{pmatrix} f_m + \begin{pmatrix} 0\cdot 42083 & 0\cdot 94167 \\ 2\cdot 40556 & 0\cdot 39444 \end{pmatrix} f_{m-1} + \begin{pmatrix} -0\cdot 01417 & -0\cdot 08749 \\ 0\cdot 13389 & -0\cdot 60278 \end{pmatrix} f_{m-2} \right) \qquad (2.11)$$

3.0 Illustrative example

Consider the non-linear system of initial value problem, considered by Liniger and Willoughby, given in the matrix form

$$y' = \begin{pmatrix} -2000 & 1000 \\ 1 & -1 \end{pmatrix} y + \begin{pmatrix} 1 \\ 0 \end{pmatrix} y_{m-2},\quad y(0) = (0,0)^T,\quad \forall x = 0(0\cdot 5)5,$$

If the theoretical solution of this system of equations is $y(x) = [y_1(x), y_2(x)]^T$. Then

$y_1(x) = A_1 e^{-0.49987505x} + B_1 e^{-2000.500125x} + 0.001$

$y_2(x) = A_2 e^{-0.49987505x} + B_2 e^{-2000.500125x} + 0.001$

where $A_1 = -5.00249997 \times 10^{-4}$, $B_1 = 4.99750002 \times 10^{-4}$

$A_2 = -1.00024993 \times 10^{-3}$, $B_2 = 2.49937494 \times 10^{-7}$

Putting $h = 0.45867(0.5)$; $R = h$; $S = 0.5h^2$, $T = (1/6)h^3$, the following tables were obtained

Table 3.01(first component)

X	Theoretical solution	New scheme	Fatunla
0.5	6.103806060378229D-04	6.103806060378229D-04	6.103806060378229D-04
1.0	6.965451636325849D-04	6.966055755021406D-04	6.955916019907959D-04
1.5	7.636543989523875D-04	7.637616668141930D-04	7.629720119974668D-04
2.0	8.159223502524445D-04	8.160662248668210D-04	8.154512027013876D-04
2.5	8.566312526725824D-04	8.568036053137039D-04	8.563245955893255D-04
3.0	8.883373367077421D-04	8.885318875901718D-04	8.881588111777582D-04
3.5	9.130316026723283D-04	9.132434436300985D-04	9.129528732616115D-04
4.0	9.322647175914462D-04	9.324900263326148D-04	9.322637157506769D-04
4.5	9.472444317943433D-04	9.474802176777583D-04	9.473039557938117D-04
5.0	9.589113705671485D-04	9.59155318028161D-04	9.590180365795390D-04

Table 3.02(first component error comparison)

x	Errors in	
	New scheme	Fatunla
0.5	-8.622486946431766D-05	-8.521099595297297D-05
1.0	-6.721650318160805D-05	-6.642684835488185D-05
1.5	-5.241182591443348D-05	-5.179680374900015D-05
2.0	-4.088125506125942D-05	-4.040224533688103D-05
2.5	-3.190063491175894D-05	-3.152755850517581D-05
3.0	-2.490610692235639D-05	-2.461553655386938D-05
3.5	-1.945842366028648D-05	-1.923211307834861D-05
4.0	-1.521550008631212D-05	-1.503923820236552D-05
4.5	-1.191088623382081D-05	-1.177350478519576D-05
5.0	-9.337091764863173D-06	-9.230170198013823D-06

Table 3.03(second component)

x	Theoretical solution	New scheme	Fatunla
0.5	2.209558701073540D-04	2.211456125614792D-04	2.195806778159415D-04
1.0	3.932419260601047D-04	3.933847491036992D-04	3.921659005532158D-04
1.5	5.274268600283223D-04	5.275330940321029D-04	5.265837945926828D-04
2.0	6.319366426302199D-04	6.320144694061078D-04	6.312751079840543D-04
2.5	7.133341039056124D-04	7.133897206896912D-04	7.128138695268057D-04
3.0	7.767304274127176D-04	7.767687925485174D-04	7.763202911717866D-04
3.5	8.261066188126192D-04	8.261315500441900D-04	8.257822349777694D-04
4.0	8.645632372366923D-04	8.645777091167462D-04	8.643056452513671D-04
4.5	8.945151797912424D-04	8.945214740043890D-04	8.943095772475774D-04
5.0	9.178432269874254D-04	9.178431557845681D-04	9.176781201335351D-04

Table 3.04(second component error comparison)

x	Errors in	
	New scheme	Fatunla
0.5	-1.897424541252636D-07	1.375192291412420D-06
1.0	-1.428230435945405D-07	1.076025506888893D-06
1.5	-1.062340037806151D-07	8.430654356395104D-07
2.0	-7.782677588783003D-08	6.615346461656636D-07
2.5	-5.561678407880609D-08	5.202343788066342D-07
3.0	-3.836513579977166D-08	4.101362409310576D-07
3.5	-2.493123157080350D-08	3.243838348497606D-07
4.0	-1.447188005392899D-08	2.575919853252021D-07
4.5	-6.294213146602261D-09	2.056025436649622D-07
5.0	7.120285730379677D-11	1.651068538903016D-07

4.0 Zero-Stability test for scheme 2.10

Definition 3. (Fatunla 1991)

The block method (2.1) is zero-stable, if and only if the roots $R_j, j = 1(1)k$ of the first characteristic polynomial $\rho(R)$ defined as $\rho(R) - \det[\Sigma A^{(i)} R^{k-i}] = 0$, satisfies $|R_j| \le 1$, and for those roots with $|R_j| = 1$, the multiplicity must not exceed two.

The first and second characteristic polynomials of (1.2) is given by the relations:

$$\rho(R) = \Sigma\alpha_j R^j; \qquad \sigma(R) = \Sigma\beta_j R^j, \qquad j = 0(1)k \qquad (4.1)$$

Now $\rho(R) = \det R^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - R\begin{pmatrix} 0 & 1.5 \\ 0 & 2 \end{pmatrix} - \begin{pmatrix} 0 & -0.5 \\ 0 & -1 \end{pmatrix} = R^2(R^2 - 2R + 1) = 0 \Leftrightarrow R = 0$ *(twice)* $\Leftrightarrow$ scheme is zero = stable. Since order of scheme = 5 > 1, Scheme is consistent and so by Dahlquist fundamental theorem of convergence, scheme (2.10) is convergent (Henrici, P(1962)[6])

Suppose scheme is explicit. Then the coefficient of the matrix $B^{(0)}$ in 2.1 will all be zero. Substituting directly in 2.1, the components of $B^{(0)}$, the following result was obtained.

$$y_m^{(0)} = \begin{pmatrix} 0 & 1\cdot 5 \\ 0 & 2 \end{pmatrix} y_{m-1} + \begin{pmatrix} 0 & -1\cdot 5 \\ 0 & -1 \end{pmatrix} y_{m-2} + h^2 \left(\begin{pmatrix} -6 & -2 \\ 0 & 8 \end{pmatrix} f_{m-1} + \begin{pmatrix} -1 & 12 \\ 0 & 16 \end{pmatrix} f_{m-2} \right) \qquad (4.2)$$

This is the resultant explicit 2-block 2-point scheme. It is of order 4 and has error constant C6 = $(-23.0375, -48.1556)^T$. This scheme can easily be used as a predictor for scheme (2.10) which itself can be used as a corrector.

This was done in this paper and both schemes were applied to the test equation y" = - 100y, given that *y*(0) =1 and *y*'(0) =10. The following table illustrates the essence of the Predictor-Corrector concept.

Table 4.1

H	**Errors in**		**Point**
	Predictor	**Corrector**	
0.001	-5.006790161132813D-05 -3.70025634765625D-04	-1.43051147609375D-05 -2.86102294921875D-06	First Second
0.0025	-3.12805175788125D-04 -2.312660217285156D-03	-8.821487426757813D-05 -1.621246337890625D-05	First Second
0.005	-1.249790191650391D-03 -9.250164031382422D-03	-3.523826599121094D-04 -6.532669067382813D-05	First Second
0.01	-5.000114440917969D-03 -3.700017929077148D-02	-1.408576965332031D-03 -2.598762512207031D-04	First Second
0.025	-3.125000000000000D-02 -2.312498092651367D-01	-8.801937103271484D-03 -1.624584197998047D-03	First Second

5.0 Conclusion

In this paper, we developed a family of numerical schemes, particularly 2-block 2-point numerical integrators of orders 5/6, by extending the ideas in Fatunla (1991, 1993). 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 2 points simultaneously.
(d) Ability to generate higher order schemes with relatively smaller step-sizes than the equivalent traditional LMM (1.2)
(e) Convergent.

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 Fatunla(1991,1993) as the illustrative example showed.

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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