Original Research Article

A Family of High Order One-Block Methods for the Solution of Stiff Initial Value Problems

Abstract.

In this paper, we construct a family of high order self-starting one-block numerical methods for the solution of stiff initial value problems (IVP) in ordinary differential equations (ODE). The Reversed Adams Moulton (RAM) methods, Generalized Backward Differentiation Formulas (GBDF) and Backward Differentiation Formulas (BDF) are used in the constructions. The E-transformation is applied to the triples and a family of self-starting methods are obtained. The family is $L-\text{stable}$ for $k \leq 7$. The numerical implementation of the methods on some stiff initial value problems are reported to show the effectiveness of the methods. The computational rate of convergence tends to the theoretical order as h tends to zero.

Keywords: stiffness, initial value problem and multistep methods,
Subject Classification: 65L04, 65L05, 65L06

1.0 Introduction

The focus of many researchers is to construct methods that are stable and with improved level of accuracy, for the solution of first and higher order ordinary differential equations. See [1, 2, 9, 10, 11, 12, 13]. In this paper, we focus on the construction of a family of block methods that exhibits the above properties (stability and accuracy) for the numerical solution $y(t)$ of the initial value problem

$$\begin{aligned} &y'(t) = f(t, y(t)); \quad y(t_0) = y_0; \quad t \in [a, b]; \\ &f : \Re \times \Re^m \rightarrow \Re^m; \quad y : \Re \rightarrow \Re^m \end{aligned} \tag{1}$$

The Reversed Adams Moulton (RAM) methods are generally written as

$$y_1 - y_0 = h_n \sum_{i=0}^{k} \beta_r f_{n+r} \tag{2}$$

(see [4]). They are therefore generally zero stable. The determination of the coefficients $\{\beta\}_{r-0}^{k}$ is done by imposing the maximum order $k+1$ on the method (2). This leads to the matrix equations

$$\begin{pmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{3} \\ . \\ . \\ . \\ \frac{1}{k+1} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1...1 \\ 0 & 1 & 2 & 3...k \\ 0 & 1 & 2^2 & 3^2...k^2 \\ . & . & . & ..... \\ . & . & . & ..... \\ . & . & . & ..... \\ 0 & 1 & 2^k & 3^k...k^k \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ . \\ . \\ . \\ \beta_k \end{pmatrix} \qquad (3)$$

which is solved simultaneously for the coefficients (see [4], [1]).

1.1 The Backward Differentiation Formulas (BDF)

A *k*-step BDF introduced in [5] is a linear multistep formula that has order *p* = *k* and error constant $C_{p+1} = \frac{-1}{k+1}$ when the coefficient of the derivative function is normalized to one. They are popular for the solution of stiff differential equations (1). They have the general formula

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h_n \beta_k f_{n+k} \qquad (4)$$

The coefficients $\{\alpha_j\}_{j=1}^{k}$ are uniquely determined by imposing the order *k* on (4) which leads to the matrix equation

$$\begin{pmatrix} 0 \\ 1 \\ 2k \\ . \\ . \\ . \\ k^k \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 . \ . \ . 1 \\ 0 & 1 & 2 & 3 . \ . \ . k \\ 0 & 1 & 2^2 & 3^2 . \ . \ . k^2 \\ . & & & \\ . & & & \\ . & & & \\ 0 & 1 & 2^k & 3^k . \ . \ . k^k \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ . \\ . \\ . \\ \alpha_k \end{pmatrix} \tag{5}$$

which are solved simultaneously. The methods have been shown in ([1], [3], [8]) to be zero stable for $k \leq 6$, and zero unstable for $k \geq 7$.

1.2 The Generalized Backward Differentiation Formulae (GBDF):

This class of methods introduced in [4] has the form

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h f_{n+j} \ , \tag{6}$$

for all $k \geq 1$, where

$$j = \begin{cases} \dfrac{k+2}{2}, & for\ even\ k, \\ \dfrac{k+1}{2}, & for\ odd\ k. \end{cases} \tag{7}$$

It implemented by coupling it with some set of initial and final additional methods. While BDF are 0-unstable, for *k* > 6, GBDF though cannot be used as single integrator, provide $0_{j,k-j} - Stable$, $A_{j,k-j} - Stable$ methods for all $k \leq 32$.

2. Construction of the new self-starting block methods

The methodology for the construction is captured in the following theorem [2]:

Theorem

Let the multi-family of LMF $\left\{\rho_k^{[j]}(R), \sigma_k^{[j]}(R)\right\}_{j=1,k=1}^{m,K}$ *be given, that is,*

$$\rho_k^{[j]}(E)y_n = h\,\sigma_k^{[j]}(E)f_n\;;\; j=1(1)m,\;\; k=1(1)K \qquad (8)$$

with $\left\{\rho_k^{[j]}, \sigma_k^{[j]}\right\}$ *for a fixed j forming a family of variable order* $p_{k,j}$ *of variable step number k. Then the resultant system of composite LMF*

$$E^i\rho_k^{[j]}(E)y_n = hE^i\sigma_k^{[j]}(E)f_n\;;\; i=0\,(1)\,k-l;\quad j=1,2,\ldots,m \qquad (9)$$

arising from the E-operator transformation of (8) *can be composed as the block method*

$$A_1Y_{n+1} + A_0Y_n = h(B_1F_{n+1} + B_0F_n)\,;\ \det(A_1)\neq 0 \qquad (10)$$

if k is chosen such that l is an integer given as

$$l = \frac{m+k(m-2)}{m-1}\;;\; m,k\geq 2 \text{ and } k-l\geq 0. \qquad (11)$$

where Y_{n+1}, Y_n; F_{n+1} *and* F_n $n=0,1,2,\ldots$ *are vectors as defined below and* A_1, A_0, B_1, B_0 *are square matrices also defined below for a fixed m.*

$$A_0 = \left(\begin{array}{c|c} O & \begin{matrix}\alpha_0^{[1]}\\ \alpha_0^{[2]}\\ .\\ .\\ .\\ \alpha_0^{[m]}\\ 0\\ .\\ .\\ .\\ 0\end{matrix}\end{array}\right)_{(2k-l)\times(2k-l)} ; \qquad B_0 = \left(\begin{array}{c|c} O & \begin{matrix}\beta_0^{[1]}\\ \beta_0^{[2]}\\ .\\ .\\ .\\ \beta_0^{[m]}\\ 0\\ .\\ .\\ .\\ 0\end{matrix}\end{array}\right)_{(2k-l)\times(2k-l)} \qquad (12)$$

$$A_1 = \begin{pmatrix}
\alpha_1^{[1]} & \cdots & \alpha_k^{[1]} & 0 & 0 & 0 & \cdots & & & 0 \\
\vdots & & & & & & & & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & & & & 0 \\
\vdots & & & & & & & & & \\
\alpha_1^{[m]} & \cdots & \alpha_k^{[m]} & 0 & \cdots & \cdots & & & & 0 \\
\alpha_0^{[1]} & \alpha_1^{[1]} & \cdots & \alpha_k^{[1]} & \cdots & \cdots & & & & 0 \\
\cdots & \cdots & \cdots & \vdots & 0 & & & & & 0 \\
 & & & & \vdots & & & & & \\
\vdots & \vdots & \cdots & \cdots & 0 & & & & & \cdots \\
\alpha_0^{[m]} & \alpha_1^{[m]} & & \alpha_k^{[m]} & 0 & & & & & \cdots \\
0 & \alpha_0^{[1]} & \alpha_1^{[1]} & & \alpha_k^{[1]} & & & & & \cdots \\
0 & \cdots & \cdots & \cdots & \cdots & & & & & \\
 & \cdots & \cdots & \cdots & \cdots & & & & & \\
 & \cdots & \cdots & \cdots & \cdots & 0 & & & & \\
 & \alpha_0^{[m]} & \alpha_1^{[m]} & \cdots & \alpha_k^{[m]} & & & & & \\
 & \cdots & \cdots & & \cdots & & & & & \\
\cdots & \cdots & \cdots & & \cdots & & & \cdots & & \\
\cdots & \cdots & \cdots & & \cdots & & \cdots & \cdots & 0 & \\
\cdots & & & & & & \alpha_0^{[1]} & & \alpha_k^{[1]} & \\
 & & & & & & \cdots & & \cdots & \\
 & & & & & & \cdots & & \cdots & \\
 & & & & & & \vdots & & \vdots & \\
0 & \cdots & \cdots & & & & 0 \quad \alpha_0^{[m]} & \cdots & \alpha_k^{[m]} &
\end{pmatrix}_{(2k-l)\times(2k-l)}$$

$$B_1 = \begin{pmatrix}
\beta_1^{[1]} & \cdots & \beta_k^{[1]} & 0 & 0 & 0 & \cdots & & & 0 \\
\vdots & & & & & & & & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & & & & 0 \\
\vdots & & & & & & & & & \\
\beta_1^{[m]} & \cdots & \beta_k^{[m]} & 0 & \cdots & \cdots & & & & 0 \\
\beta_0^{[1]} & \beta_1^{[1]} & \cdots & \beta_k^{[1]} & \cdots & \cdots & & & & 0 \\
\cdots & \cdots & \cdots & \vdots & 0 & & & & & 0 \\
 & & & & \vdots & & & & & \\
\vdots & \vdots & \cdots & \cdots & 0 & & & & & \cdots \\
\beta_0^{[m]} & \beta_1^{[m]} & & \beta_k^{[m]} & 0 & & & & & \cdots \\
0 & \beta_0^{[1]} & \beta_1^{[1]} & & \beta_k^{[1]} & & & & & \cdots \\
0 & \cdots & \cdots & \cdots & \cdots & & & & & \\
 & \cdots & \cdots & \cdots & \cdots & & & & & \\
 & \cdots & \cdots & \cdots & \cdots & 0 & & & & \\
 & \beta_0^{[m]} & \beta_1^{[m]} & \cdots & \beta_k^{[m]} & & & & & \\
 & \cdots & \cdots & & \cdots & & & & & \\
\cdots & \cdots & \cdots & & \cdots & & & \cdots & & \\
\cdots & \cdots & \cdots & & \cdots & & \cdots & \cdots & 0 & \\
\cdots & & & & & & \beta_0^{[1]} & & \beta_k^{[1]} & \\
 & & & & & & \cdots & & \cdots & \\
 & & & & & & \cdots & & \cdots & \\
 & & & & & & \vdots & & \vdots & \\
0 & \cdots & \cdots & & & & 0 \quad \beta_0^{[m]} & \cdots & \beta_k^{[m]} &
\end{pmatrix}_{(2k-l)\times(2k-l)}$$

$$Y_{n+1} = (y_{n+1}, y_{n+2}, ..., y_{n+2k-l})^T ; \quad Y_n = (y_{n-2k+l+1}, y_{n-2k+l+2}, ..., y_{n-1}, y_n)^T ;$$
$$F_{n+1} = (f_{n+1}, f_{n+2}, ..., f_{n+2k-l})^T ; \quad F_n = (f_{n-2k+l+1}, f_{n-2k+l+2}, ..., f_{n-1}, f_n)^T \quad (13)$$
$$n = 0, 1, 2, ...$$

Proof:

Notice that the *E*-operator is effectively applied *k-l* times on the system of LMF $\left\{\rho_k^{[j]},\ \sigma_k^{[j]}\right\}_{k,j}$. Thus there are 2*k-l* unknown solution points captured in the block of solution $Y_{n+1} = (y_{n+1}, y_{n+2}, ..., y_{n+2k-l})^T$. By this the block definition in (11) is realized if the coefficient matrices A_1, A_0, B_1, B_0 are square matrices of dimension $(2k-l)\times(2k-l)$.

This simply imply that $m + m(k-l) = 2k-l$ so that *l* is as in (12) and for a fixed *m* the *k* is then chosen such that $k - l \geq 0$

In particular:

(1.) $m = 2$; $l = 2$ $k = 2, 3, 4, ...$

(2.) $m = 3$; $l = \dfrac{k+3}{2}$; $k = 3, 5, 7, ...$

(3.) $m = 4$; $l = \dfrac{4+2k}{3}$; $k = 4, 7, 10, 13, ...$

When $k - l = 0$, the method requires no shifting, this is so if $m=k$. However, the case of interest in this paper is when *m* = 3.

Consider the triple of *k*-step LMF defined by $[\rho_1, \sigma_1]$, $[\rho_2, \sigma_2]$ and $[\rho_3, \sigma_3]$ Shifting this (*k-l*) times, where $l = \dfrac{k+3}{2}$, we have a set of 2*k-l* equations in 2*k-l* unknowns which can be written in the block form (10).

3 Stability of the Implicit Block Methods

When (10) is applied to test equation

$$y' = \lambda y \text{ , } \mathrm{Re}(\lambda) < 0 \quad (14)$$

it yields the characteristics equation.

$$\pi(R,z) = \det(A_1 R + A_0 - z(B_1 R + B_0)) \tag{15}$$

The region of absolute stability R_A associated with (10) is the set

$$R_A = \{z : |R_j(z)| \le 1,\ j = 1(1)k\} \tag{16}$$

If we let $z \to 0$ in (15), the difference system becomes

$$\pi(R,0) = \det(A_1 R + A_0) \tag{17}$$

All the proposed block methods can be cast in the form

$$A_1 Y_{n+1} + \hat{a} y_n = h(B_1 F_{n+1} + \hat{b} f_n) \tag{18}$$

where

$$\hat{a} = \begin{pmatrix} \alpha_0^{[1]} \\ \alpha_0^{[2]} \\ . \\ . \\ . \\ \alpha_0^{[m]} \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}_{(2k-l)\times 1} \quad ; \quad \hat{b} = \begin{pmatrix} \beta_0^{[1]} \\ \beta_0^{[2]} \\ . \\ . \\ . \\ \beta_0^{[m]} \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}_{(2k-l)\times 1} \tag{19}$$

Note that for all the block methods, $A_1^{-1}\hat{a} = (1\,1\,1 \ldots 1)^T = e$

implying that

$$A_1^{-1}A_0 = \left(\begin{array}{c|c} O & \begin{matrix}1\\1\\\cdot\\\cdot\\1\end{matrix}\end{array}\right) = (O \quad e)$$

To see this, assume order $p \geq 1$ for all the LMF that constitute the block, then by consistency,

$$A_1 e + \hat{a} = 0 \tag{20}$$

where $e = (1\,1\,1\ldots1)^T$. From (20) it follows that

$$A_1^{-1}\hat{a} = -e \tag{21}$$

The above ensures zero-stability of the implicit block methods (10). Method (10) applied to test equation can also be written as

$$Y_{n+1} = M(z)Y_n, \quad z = \lambda h \tag{22}$$

where

$$M(z) = (I - zA_1^{-1}B_1)^{-1}(zA_1^{-1}B_0 - A_1^{-1}A_0) \tag{23}$$

is the amplification matrix. If as *z* tends to infinity (23) tends to zero (that is $M(\infty) = 0$), it means that an A-stable (10) is *L*-stable. If we take $[\rho_1, \sigma_1]$, $[\rho_2, \sigma_2]$ and $[\rho_3, \sigma_3]$ to be RAM, GBDF and BDF respectively, then the coefficients of order 3 method

$$A_1 = \begin{pmatrix} 1 & 0 & 0 \\ -1 & \frac{1}{2} & \frac{1}{3} \\ \frac{3}{2} & -3 & \frac{11}{6} \end{pmatrix}; A_0 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & -\frac{1}{3} \end{pmatrix}; B_0 = \begin{pmatrix} 0 & 0 & \frac{5}{12} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; B_1 = \begin{pmatrix} \frac{2}{3} & -\frac{1}{12} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Coefficients of order 5 method

$$A_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & -1 & \frac{1}{3} & \frac{1}{2} & -\frac{1}{20} & 0 \\ \frac{5}{4} & -\frac{10}{3} & 5 & -5 & \frac{137}{60} & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{30} & \frac{1}{4} & -1 & \frac{1}{3} & \frac{1}{2} & -\frac{1}{20} \\ -\frac{1}{5} & \frac{5}{4} & -\frac{10}{3} & 5 & -5 & \frac{137}{60} \end{pmatrix}; A_0 = \begin{pmatrix} & -1 \\ O_{3X5} & -\frac{1}{30} \\ & -\frac{1}{5} \\ O_{3X5} & O_{3X1} \end{pmatrix};$$

$$B_0 = \begin{pmatrix} O_{1X5} & \frac{251}{720} \\ O_{5X5} & O_{5X1} \end{pmatrix}; B_1 = \begin{pmatrix} \frac{323}{360} & -\frac{11}{30} & \frac{53}{360} & -\frac{19}{720} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ \frac{251}{720} & \frac{323}{360} & -\frac{11}{30} & \frac{53}{360} & -\frac{19}{720} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Coefficients of order 7 method

$$A_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{15} & \frac{3}{10} & -1 & \frac{1}{4} & \frac{3}{5} & -\frac{1}{10} & \frac{1}{105} & 0 & 0 \\ \frac{7}{6} & -\frac{21}{5} & \frac{35}{4} & -\frac{35}{3} & \frac{21}{2} & -7 & \frac{363}{140} & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{140} & -\frac{1}{15} & \frac{3}{10} & -1 & \frac{1}{4} & \frac{3}{5} & -\frac{1}{10} & \frac{1}{105} & 0 \\ -\frac{1}{7} & \frac{7}{6} & -\frac{21}{5} & \frac{35}{4} & -\frac{35}{3} & \frac{21}{2} & -7 & \frac{363}{140} & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{140} & -\frac{1}{15} & \frac{3}{10} & -1 & \frac{1}{4} & \frac{3}{5} & -\frac{1}{10} & \frac{1}{105} \\ 0 & -\frac{1}{7} & \frac{7}{6} & -\frac{21}{5} & \frac{35}{4} & -\frac{35}{3} & \frac{21}{2} & -7 & \frac{363}{140} \end{pmatrix};$$

$$A_0 = \begin{pmatrix} & -1 \\ & \frac{1}{140} \\ O_{3x8} & \\ & -\frac{1}{7} \\ O_{6x8} & O_{6x1} \end{pmatrix}; B_0 = \begin{pmatrix} O_{1x8} & \frac{19087}{60480} \\ O_{8x8} & O_{8x1} \end{pmatrix};$$

$$B_1 = \begin{pmatrix} \frac{2713}{2520} & -\frac{15487}{20160} & \frac{586}{945} & -\frac{6737}{20160} & \frac{263}{2520} & -\frac{863}{60480} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \frac{19087}{60480} & \frac{2713}{2520} & -\frac{15487}{20160} & \frac{586}{945} & -\frac{6737}{20160} & \frac{263}{2520} & -\frac{863}{60480} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{19087}{60480} & \frac{2713}{2520} & -\frac{15487}{20160} & \frac{586}{945} & -\frac{6737}{20160} & \frac{263}{2520} & -\frac{863}{60480} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The stability function $P(z)$ is

$$P(z) = Det[I_k R - M(z)] = R^{k-1}(R - D(z)) \quad (24)$$

The stability domain *S* of this family is

$$S = \{z \in \mathbb{C} : |R(z)| \leq 1\} \quad (25)$$

The $D(z)$ (the only non-zero value of *R*(*z*)) for this family of methods are given as a rational function $D(z) = \frac{P(z)}{Q(z)}$. where P{z) and Q(z) are polynomials.

Case of order p = 3

$$D(z) = \frac{138 + 168z + 61z^2}{138 - 246z + 178z^2 - 48z^3}$$

Case of order p = 5

$$D(z) = \frac{(645924960 + 1787505120z + 2201902944z^2 + 1527877926z^3 + 577756622z^4 + 20012481z^5)}{(645924960 - 2088044640z + 3103521504z^2 - 2761746138z^3 + 1574505578z^4 - 543891495z^5 + 87044400z^6)}$$

Case of order p = 7

$$D(z) = 8516516147374800384 0 + 44020513921597091424 00 z + 93120558823712493558 00 z^2 + 122745780100367618490 00 z^3 + 111007963694668658748 24 z^4 + 705016586652036468268 0 z^5 + 295534823315859279959 5 z^6 + 519376147126246691525 z^7 + 144916833633604500 0 z^8$$

$$Q(z) = 8516516147374800384 0 - 44644350611040228921 60 z + 95927823926206612297 20 z^2 - 129484106678966445525 60 z^3 + 1[illegible]38139385652807891884 z^4 - 85157292608334322219 44 z^5 + 44314384729600538124 04 z^6 + [illegible]527333808945190124 0 z^7 + 41588079912131062800 0 z^8 - 51054324417768672000 z^9$$

Definition1: A block method is said to be pre-stable if the roots of $Q(z)$ are contained in C^+.

For the cases of orders 3, 5 and 7 above $D(z)$ has no negative pole on C^-. In all the cases, the roots of $Q(z)$ are contained in C^+ as shown below:

roots for case: *k*=3 are $\{\{z \to 1.0187340384857744 - 0.8263451688443794i\}, \{z \to 1.0187340384857744 + 0.8263451688443794i\}, \{z \to 1.6708652563617843\}\}$

roots for case: *k*=5 are $\{\{z \to 0.5496503163387506 - 1.3267991841349167i\}, \{z \to 0.5496503163387506 + 1.3267991841349167i\}, \{z \to 1.151541041151053 - 0.6310368906999217i\}, \{z \to 1.151541041151053 + 0.6310368906999217i\}, \{z \to 1.4230274032805632 - 0.24822115565736874i\}, \{z \to 1.4230274032805632 + 0.24822115565736874i\}\}$

roots for case: *k*=7 are $\{\{z \to 0.12805543041947612 - 1.6041775714692936i\}, \{z \to 0.12805543041947612 + 1.6041775714692936i\}, \{z \to 0.7828629304247531 - 0.9771613463405875i\}, \{z \to 0.7828629304247531 + 0.9771613463405875i\}, \{z \to 1.052641898979391 - 0.30282200428785017i\}, \{z \to 1.052641898979391 + 0.30282200428785017i\}, \{z \to 1.2966180420834268 - 0.8693941685370542i\}, \{z \to 1.2966180420834268 + 0.8693941685370542i\}, \{z \to 1.6254920361214837\}\}$

The one step block method is *A*-stable if and only if it is stable on the imaginary axis (*I*-stable): $D(iy) \leq 1$ for all $y \in \Re$, and *D*(z) is analytic for $D(z) < 0$ (i.e., $Q(z)$ does not have roots with negative or zero real parts), *I*-stability is equivalent to the fact that the Norsett polynomial defined by

$$E(y) = |Q(iy)|^2 - |P(iy)|^2 = Q(iy)Q(-iy) - P(iy)P(-iy) \qquad (26)$$

satisfies $E(y) > 0$ for all $y \in \Re$, see [7]. In each of the cases of order *p* = 3, 5, 7, (26) is satisfied and $D(z) \to 0$ as $z \to \infty$ implying that the methods are *L-stable* for $k \leq 7$

4 Numerical implementation

Problem 1: (cf: [4])

$$y' = \begin{pmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{pmatrix} y; \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

The theoretical solution of the problem is:

$$y(t) = \frac{1}{2}\begin{pmatrix} e^{-2t} + e^{-40t}(\cos(40t) + \sin(40t)) \\ e^{-2t} - e^{-40t}(\cos(40t) + \sin(40t)) \\ 2e^{-40t}(\sin(40t) - \cos(40t)) \end{pmatrix}$$

Problem 2: (cf: [6])

$$\frac{dy}{dt} = f(y); \quad t \in [0, T]$$

The function *f* is defined by

$$f(y) = \begin{pmatrix} -k_1 y_1 + k_2 y_2 y_3 \\ k_1 y_1 - k_2 y_2 y_3 - k_3 y_2^2 \\ k_3 y_2^2 \end{pmatrix}; \; y(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$k_1 = 0.04; \; k_2 = 10^4; \; k_3 = 3.10^7$$

Problem 1 is solved using order p=3, 5, 7 and 9. The error and rate of computational convergence are displayed in table 1. It can be seen that the rate of computational convergence is tending towards the theoretical order as *h* tends to 0 except for the method of order 9 which exhibit order reduction The error in order 3 when used to solve problem 1 is plotted against the step size *h* and displayed in figure 1.

Table 1: Error and order of convergence of RAM/GBDF/BDF *p*=3, 5, 7, 9

H	*Error*	*rate*	*Error*	*Rate*	*Error*	*Rate*	*Error*	*rate*
1e-2	2.697e-02		6.136e-02		4.641e-02		7.166e-02	
5e-3	4.879e-03	2.47	2.735e-03	4.49	3.231e-03	3.84	1.047e-03	6.10
2.5e-3	6.510e-04	2.91	7.608e-05	5.17	3.889e-05	6.38	6.234e-06	7.39
1.25e-3	8.363e-05	2.96	2.357e-06	5.01	3.909e-07	6.64	3.803e-08	7.36
6.25e-4	1.061e-05	2.98	7.192e-08	5.03	3.431e-09	6.83	2.753e-10	7.11

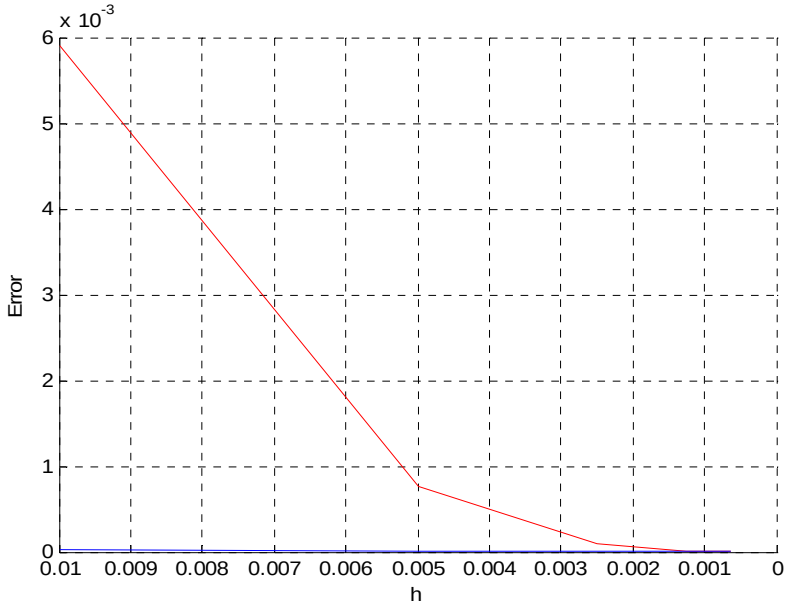

Figure 1: Error in the proposed method of order *p*=3 for problem 1 versus *h*.

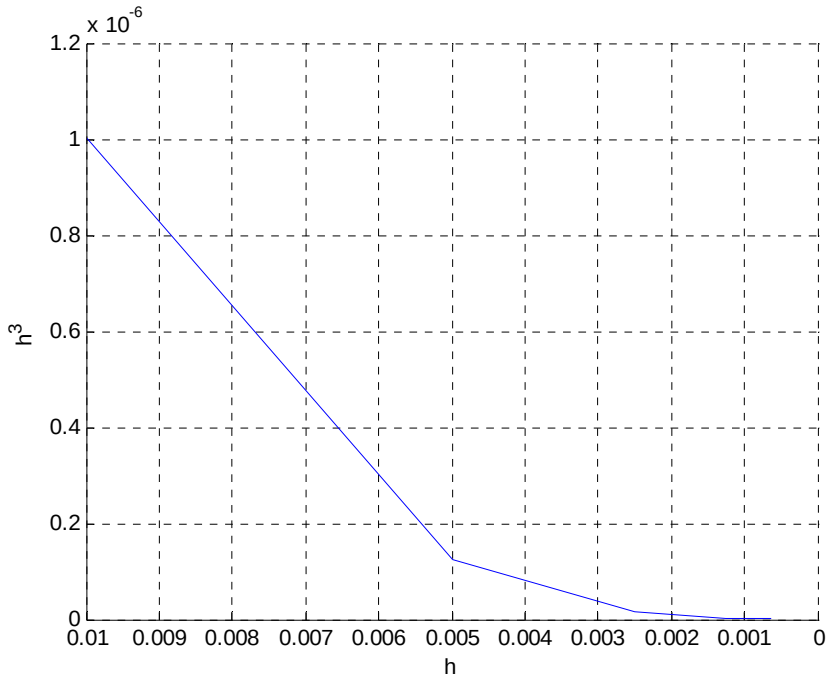

Figure 2: Slope for order 3 method.

Comparing figures 1 and 2, it is observed that the computational convergence rate and the theoretical rate of convergence have the same slope for order 3 method.

Problem 2 is a Chemical Kinetics Problem. It is solved using order 5 of the proposed method and constant step size *h* = 0.0001. The error tolerance for accuracy in the Newton-Raphson iteration is set at 10^{-2}. The errors in the table 2 are the maximum absolute values of the difference between approximate solution of the proposed method and that of MATLAB ODE15s (which is assumed to be the exact solution of the problem).

Table 2: Errors from proposed method, k=5; p=5 when applied to problem 2

T	2.00	5.00	7.5	10.00
Errors	2.30e-006	4.20e-006	4.41e-005	7.19e-005

5 Conclusion:

We have constructed a family of high order self-starting one-block methods using multistep triple. This family is zero stable for all $k \geq 3$, *I*-stable for $k \leq 7$ and exhibit order reduction for $k = 9$. The numerical examples considered showed that the methods are comparable to the existing ones.

Ethical: NA

Consent: NA

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