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

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Authors' contributions

This work was carried out in collaboration among all authors. Authors IJA and PO designed the study and wrote the first draft of the manuscript. Authors IJA and KU managed the analyses and implementation of the study. Author IJA managed the literature searches. All authors read and approved the final manuscript.

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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 (BDF) 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-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.

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1 Introduction

(1)

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 [1,2,3,4,5,6,7]. 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

$$y'(t) = f(t, y(t)); \quad y(t_0) = y_0; \quad t \in [a, b];$$

$$f: \Re \times \Re^m \to \Re^m; \quad y: \Re \to \Re^m$$
(1)

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

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

(see [8]). 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

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

which is solved simultaneously for the coefficients (see [8,1]).

1.1 The backward differentiation formulas (BDF)

A k-step BDF introduced in [9] 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

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

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

which are solved simultaneously. The methods have been shown in [1,10,11] to be zero stable for $k \le 6$, and zero unstable for $k \ge 7$.

1.2 The generalized backward differentiation formulae (GBDF)

This class of methods introduced in [8] has the form

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

for all $k \ge 1$, where

$$j = \begin{cases} \frac{k+2}{2}, & \text{for even } k, \\ \frac{k+1}{2}, & \text{for odd } k. \end{cases}$$
⁽⁷⁾

It implemented by coupling it with some set of initial and final additional methods. While BDF are 0unstable, 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 $k \le 32$.

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 $\left\{
ho_k^{[j]}(R), \sigma_k^{[j]}(R) \right\}_{j=1,k=1}^{m,K}$ be given, that is,

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

with $\{\rho_k^{[j]}, \sigma_k^{[j]}\}\$ 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

$$E^{i}\rho_{k}^{[j]}(E)y_{n} = hE^{i}\sigma_{k}^{[j]}(E)f_{n}; \quad i = 0(1)k - l; \quad j = 1, 2, ..., m$$
(9)

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

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

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

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

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

$$A_{0} = \begin{pmatrix} & & \alpha_{0}^{[1]} \\ & & \alpha_{0}^{[2]} \\ & & \ddots \\ & & \ddots \\ & & \ddots \\ & & \alpha_{0}^{[m]} \\ O & & 0 \\ & & \ddots \\ & & & 0 \end{pmatrix}_{(2k-l)\times(2k-l)}$$
(12)



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

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

$$n = 0, 1, 2, ...$$
(13)

Proof:

Notice that the *E*-operator is effectively applied *k-l* times on the system of LMF $\{\mathcal{P}_{k}^{[j]}, \sigma_{k}^{[j]}\}_{k,j}$. Thus there are 2k-*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 $k - l \ge 0$

In particular:

(1.)
$$m = 2$$
; $l = 2$ $k = 2, 3, 4, ...$
(2.) $m = 3$; $l = \frac{k+3}{2}$; $k = 3, 5, 7, ...$
(3.) $m = 4$; $l = \frac{4+2k}{3}$; $k = 4, 7, 10, 13, ...$

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 $l = \frac{k+3}{2}$, 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

$$y' = \lambda y, \operatorname{Re}(\lambda) < 0 \tag{14}$$

it yields the characteristics equation.

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

The region of absolute stability $R_{\scriptscriptstyle A}$ associated with (10) is the set

$$R_{A} = \{ z : \left| R_{j}(z) \right| \le 1, \ j = 1(1)k \}$$
⁽¹⁶⁾

If we let $z \rightarrow 0$ 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

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

Where

$$\hat{a} = \begin{pmatrix} \alpha_{0}^{[1]} \\ \alpha_{0}^{[2]} \\ \vdots \\ \vdots \\ \alpha_{0}^{[m]} \\ 0 \\ \vdots \\ \vdots \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}_{(2k-l)\times 1} , \hat{b} = \begin{pmatrix} \beta_{0}^{[1]} \\ \beta_{0}^{[2]} \\ \vdots \\ \beta_{0}^{[m]} \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}_{(2k-l)\times 1}$$
(19)

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

$$A_{1}^{-1}A_{0} = \begin{pmatrix} & 1 \\ & 1 \\ O & \cdot \\ & \cdot \\ & \cdot \\ & \cdot \\ & 1 \end{pmatrix} = \begin{pmatrix} O & e \end{pmatrix}$$

implying that

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

$$A_{\rm l}e + \hat{a} = 0 \tag{20}$$

where $e = (1 \ 1 \ 1 \dots 1)^{T}$. 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

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

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

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

Coefficients of order 7 method

The stability function P(z) is

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

The stability domain S of this family is

$$S = \{z \in \mathbf{C} : |R(z)| \le 1\}$$
⁽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

$$985165161473748003840 + 4402051392159709142400z + 9312055882371249355800z^{2} + 12274578010036761849000z^{3} + 11100796369466865874824z^{4} + 7050165866520364682640z^{5} + 2955348233158592799595z^{6} + 519376147126246691525z^{7} + 1449168336336045000z^{8} - 2955348233158592799595z^{6} + 519376147126246691525z^{7} + 1449168336336045000z^{8} - 12948410667896644552560z^{3} + 12238139385652807891884z^{4} - 8515729260833432221944z^{5} + 4431438472960053812404z^{6} - 1675273338089451901240z^{7} + 415880799121310628000z^{8} + 51054324417768672000z^{9}$$

Definition 1: 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 \rightarrow 1.0187340384857744 - 0.8263451688443794i}, {z \rightarrow 1.0187340384857744 + 0.8263451688443794i}, {z \rightarrow 1.6708652563617843}
```

```
roots for case: k=5 are

{\{z \rightarrow 0.5496503163387506 - 1.3267991841349167i\}, \{z \rightarrow 0.5496503163387506 + 1.3267991841349167i\}, \{z \rightarrow 1.151541041151053 - 0.6310368906999217i\}, \{z \rightarrow 1.151541041151053 + 0.6310368906999217i\}, \{z \rightarrow 1.4230274032805632 - 0.24822115565736874i\}, \{z \rightarrow 1.4230274032805632 + 0.24822115565736874i\}
```

```
roots for case: k=7 are

{{z \rightarrow 0.12805543041947612 - 1.6041775714692936i}, {z \rightarrow 0.12805543041947612 + 1.6041775714692936i}, {z \rightarrow 0.7828629304247531 - 0.9771613463405875i}, {z \rightarrow 0.7828629304247531 + 0.9771613463405875i}, {z \rightarrow 1.052641898979391 - 0.30282200428785017i}, {z \rightarrow 1.052641898979391 + 0.30282200428785017i}, {z \rightarrow 1.2966180420834268 - 0.8693941685370542i}, {z \rightarrow 1.2966180420834268 + 0.8693941685370542i}, {z \rightarrow 1.6254920361214837}
```

The one step block method is A-stable if and only if it is stable on the imaginary axis (I-stable): $D(iy) \le 1$ 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

$$E(y) = |Q(iy)|^{2} - |P(iy)|^{2} = Q(iy)Q(-iy) - P(iy)P(-iy)$$
(26)

satisfies E(y) > 0 for all $y \in \Re$, see [12]. 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 $k \le 7$

4 Numerical Implementation

Problem 1: (cf: [8])

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

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: [13])

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

The function f is defined by

$$f(y) = \begin{pmatrix} -k_1y_1 + k_2y_2y_3 \\ k_1y_1 - k_2y_2y_3 - k_3y_2^2 \\ k_3y_2^2 \end{pmatrix}; \ y(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$
$$k_1 = 0.04; \ k_2 = 10^4; \ k_3 = 3.10^7$$

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 Fig. 1.

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

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

x 10⁻³



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



Fig. 2. Slope for order 3 method

Comparing Figs. 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

Т	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 $k \ge 3$, *l*-stable for $k \le 7$ and exhibit order reduction for k = 9. The numerical examples considered showed that the methods are comparable to the existing ones.

Competing Interests

Authors have declared that no competing interests exist.

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