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Original Research

Second derivative off-node block adaptive backward differentiation formulae for stiff initial value problems

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Abstract

The quest for more efficient schemes that handle stiff initial value problems (IVPs) has led to the emergence of new families of methods. Amongst these methods is the Adaptive Backward Differentiation Formula (A-BDF), which is a variant of the Backward Differentiation Formula (BDF). In this study, a family of Block Adaptive Backward Differentiation Formulae is considered and it is developed through Taylor series expansion and the method of undetermined coefficients. The methods constructed herein are of order p = 2k. Numerical experiments on standard test problems show that the proposed methods produced more accurate solutions than existing methods in the literature.

Keywords: Adaptive BDF, A-stability, Block methods, Off-node methods, Stiff IVPs

1. Introduction

The understanding of systems' dynamics depends solely on the availability of solutions of differential equations that describe the models which represent the systems. Mathematical models that describe phenomena such as mechanical systems, electrical circuits, vibrating structures, chemical reaction kinetics, population dynamics and economic growth, will be of no use if these models are insoluble. Most initial value problems (IVPs) that describe real-life phenomena possess solutions that are characterised by wide varying decay rates, thereby making it difficult for numerical methods to track solution trajectories. This is due to the fact that most methods are constrained to adopt very small step lengths in the computation process. IVPs whose solution components decay at very wide rates are known as stiff and require special numerical methods to handle them. In Ref. [1], attempts were made to illustrate the idea of stiffness through transient and non-transient (steady) parts of a solution. Assume a linear system with constant coefficients given as:

$$y' = f(t, y(t)) = Ay + \vartheta(t), \quad f: \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m, \quad y: \mathbb{R} \to \mathbb{R}^m, \quad y(t_0) = y_0, \tag{1}$$

where A is an $m\times m$ matrix with real coefficients with all its distinct eigenvalues, λ_j, $j=1,2,\cdots,m$, contained in the open left half plane and the stiffness ratio φ being large.

Definition

The system of IVPs (1) is said to be stiff over the finite interval $a\le t\le b$, if for every t in the interval, the eigenvalues $\left\{\lambda_j, j=1,2,\cdots,m\right\}$ of the Jacobian matrix $J=\dfrac{\partial f}{\partial y}$ satisfy the following conditions:

i.) $\operatorname{Re}(\lambda_j)<0, j=1,2,\cdots,m$, where $\operatorname{Re}(\lambda_j)$ is the real part of the complex root $\lambda_j(t)$.

ii.) the ratio $\varphi=\dfrac{\max\limits_j|\lambda_i|}{\min\limits_j|\lambda_i|}>>1$, for $i=1,2,\cdots,m,\quad j=1,2,\cdots,m$ holds, [1], [2], [3].

The general solution of (1) is given by:

$$y(t)=\sum_{j=1}^{m}c_j\,e^{\lambda_j t}\eta_j+\vartheta(t) \tag{2}$$

where $c_j,\ j=1,2,\cdots,m$ are arbitrary constants, $\eta_j,\ j=1,2,\cdots,m$ are the eigenvectors corresponding to the eigenvalues $\lambda_j,\ j=1,2,\cdots,m$, and $\vartheta(t)$ is the particular solution of (1). The general solution (2) is made up of two parts – transient and steady-state solutions, [3]. The transient part of the solution $\sum_{j=1}^{m}c_j\,e^{\lambda_j t}\eta_j$ tends to 0 faster as t tends to ∞ for $\operatorname{Re}(\lambda_j)<0$, so that the solution $y(t)$ approaches $\vartheta(t)$ asymptotically as t tends to ∞. As $t\to\infty$, the transient part decays exponentially if $\lambda_j\in\mathbb{R}$ and sinusoidal if $\lambda_j\in\mathbb{C}$.

In the literature, block methods are shown to possess the capacity to generate solutions simultaneously at various points and were developed in Refs. [4], [5], [6], [7]. In Ref. [8], a family of methods referred to as Adaptive Backward Differentiation Formulae (A-BDF) for the numerical integration of stiff initial value problems were introduced. Modifications of A-BDF were carried out in Refs. [9] and [10]. Hence, this study is on the development of a family of one-step block adaptive backward differentiation formulae with intermediate points for the solution of stiff IVPs.

2. Development of Proposed Methods

Consider the second derivative adaptive backward differentiation formula

$$\sum_{j=0}^{k}(1-\gamma)a_{ij}y_{n+j}=hb_{ii}(f_{n+i}-\gamma f_{n+i-1})+h^2d_{ii}(f'_{n+i}-\delta f'_{n+i-1}), \tag{3}$$

where $-1\le\gamma\le1$, $-1\le\delta\le1$, and a_{ij}, b_{ij}, $i,j=1,2,\cdots,k$, are parameters to be determined, k is the step number, h is the step length and γ, δ the blend parameters.
Set $i=k=1$ to obtain

$$(1-\gamma)a_{10}y_n+(1-\gamma)a_{11}y_{n+1}=hb_{11}(f_{n+1}-\gamma f_n)+h^2d_{11}(f'_{n+1}-\delta f'_n) \tag{4}$$

The method (4) is generalised to block formulation as:

$$A_1Y_{m-1}+I_kY_m=h\,B_0F_m-h\gamma\,B_1F_{m-1}+h^2\,D_0F'_m-h^2\delta\,D_1F'_{m-1}. \tag{5}$$

where I_k is a $k \times k$ dimensional matrix.

Let y_{n+v_j} be approximation to $y(t_{n+v_j})$ at t_{n+v_j}, where $v_j = \frac{j}{k}$, $j = (0,1,2,\cdots,k)$ is the scaling factor and the solution y_{n+v_j} is within an interval [0, 1] and $v_k = 1$, [11], [12].

The method (5) is defined by $Y_m = \left(y_{n-1+v_1}, y_{n-1+v_2}, \cdots, y_n\right)^T$, $F_m = \left(f_{n-1+v_1}, f_{n-1+v_2}, \cdots, f_n\right)^T$, $F_{m+1} = \left(f_{n+v_1}, f_{n+v_2}, \cdots, f_{n+v_k}\right)^T$, $F'_m = \left(f'_{n-1+v_1}, f'_{n-1+v_2}, \cdots, f'_n\right)^T$, $F'_{m+1} = \left(f'_{n+v_1}, f'_{n+v_2}, \cdots, f'_{n+v_k}\right)^T$.

The structure of the proposed method is specified by the matrix coefficients:

$$I_k = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}, \quad B_1 = \begin{pmatrix} 0 & 0 & \cdots & 0 & b_{10} \\ 0 & 0 & \cdots & 0 & b_{20} \\ 0 & 0 & \cdots & 0 & b_{30} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & b_{k0} \end{pmatrix}$$

$$B_0 = \begin{pmatrix} b_{11} & b_{12} & b_{13} & \cdots & b_{1k} \\ b_{21} & b_{22} & b_{23} & \cdots & b_{2k} \\ b_{31} & b_{32} & b_{33} & \cdots & b_{3k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{k1} & b_{k2} & b_{k3} & \cdots & b_{kk} \end{pmatrix}, \quad D_1 = \begin{pmatrix} 0 & 0 & \cdots & 0 & d_{10} \\ 0 & 0 & \cdots & 0 & d_{20} \\ 0 & 0 & \cdots & 0 & d_{30} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & d_{40} \end{pmatrix}, \quad D_0 = \begin{pmatrix} d_{11} & d_{12} & d_{13} & \cdots & d_{1k} \\ d_{21} & d_{22} & d_{23} & \cdots & d_{2k} \\ d_{31} & d_{32} & d_{33} & \cdots & d_{3k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d_{k1} & d_{k2} & d_{k3} & \cdots & d_{kk} \end{pmatrix},$$

The linear difference operator associated with each component of the block method (5) is given as:

$$\begin{aligned} L_i[y(t_n);h] = {} & y(t_{n+v_i}) - y(t_n) + h\gamma b_{i1} f(t_n, y(t_n)) - h b_{i1} f(t_{n+v_1}, y(t_{n+v_1})) - \cdots - h b_{ik} f(t_{n+v_k}, y(t_{n+v_k})) + \\ & h^2 \delta d_{i1} f'(t_n, y(t_n)) - h^2 d_{i1} f'(t_{n+v_1}, y(t_{n+v_1})) - \cdots - h^2 d_{ik} f'(t_{n+v_k}, y(t_{n+v_k})). \end{aligned}$$

Invoking the Taylor's series expansion about t_n for each component and collecting the coefficients, and using the method of undetermined coefficients, elements of the block matrices are determined.

2.1 Development of two-point method

To construct the two-point method, the matrix difference equation in compact form is given as:

$$\begin{aligned} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y(t_{n+\frac{1}{2}}) \\ y(t_{n+1}) \end{pmatrix} = {} & \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y(t_{n-\frac{1}{2}}) \\ y(t_n) \end{pmatrix} + \gamma h \begin{pmatrix} 0 & b_{10} \\ 0 & b_{20} \end{pmatrix} \begin{pmatrix} y'(t_{n-\frac{1}{2}}) \\ y'(t_n) \end{pmatrix} + h \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} y'(t_{n+\frac{1}{2}}) \\ y'(t_{n+1}) \end{pmatrix} \\ & + \delta h^2 \begin{pmatrix} 0 & d_{10} \\ 0 & d_{20} \end{pmatrix} \begin{pmatrix} y''(t_{n-\frac{1}{2}}) \\ y''(t_n) \end{pmatrix} + h^2 \begin{pmatrix} d_{11} & d_{12} \\ d_{22} & d_{22} \end{pmatrix} \begin{pmatrix} y''(t_{n+\frac{1}{2}}) \\ y''(t_{n+1}) \end{pmatrix} \end{aligned} \quad (6)$$

Let the exact solution of (1) be assumed sufficiently differentiable. The linear difference operators associated with the component schemes are:

$$\begin{aligned} L_1[y(t_n),h] &= y(t_n+\tfrac{1}{2}h)-y(t_n)+h\gamma b_{11}y'(t_n)-hb_{11}y'(t_n+\tfrac{1}{2}h)-hb_{12}y'(t_n+h) \\ &\quad +h^2\delta d_{11}y''(t_n)-h^2d_{11}y''(t_n+\tfrac{1}{2}h)-h^2d_{12}y''(t_n+h), \end{aligned} \tag{7}$$

$$\begin{aligned} L_2[y(t_n),h] &= y(t_n+h)-y(t_n)+h\gamma b_{21}y'(t_n)-hb_{21}y'(t_n+\tfrac{1}{2}h)-hb_{22}y'(t_n+h) \\ &\quad +h^2\delta d_{21}y''(t_n)-h^2d_{21}y''(t_n+\tfrac{1}{2}h)-h^2d_{22}y''(t_n+h). \end{aligned} \tag{8}$$

Invoking the Taylor series expansion about t_n and collecting the coefficients in terms of *h* in (7) gives

$$\left.\begin{array}{ll} h^0: & 1-1 \\ h^1: & \frac{1}{2}+\gamma b_{11}-b_{11}-b_{12} \\ h^2: & \frac{1}{8}-\frac{1}{2}b_{11}-b_{12}+\delta d_{11}-d_{11}-d_{12} \\ h^3: & \frac{1}{48}-\frac{1}{8}b_{11}-\frac{1}{2}b_{12}-\frac{1}{2}d_{11}-d_{12} \\ h^4: & \frac{1}{384}-\frac{1}{48}b_{11}-\frac{1}{6}b_{12}-\frac{1}{8}d_{11}-\frac{1}{2}d_{12} \end{array}\right\} \tag{9}$$

Invoking the Taylor series expansion about t_n and collecting the coefficients in (8) gives

$$\left.\begin{array}{ll} h^0: & 1-1 \\ h^1: & 1+\gamma b_{21}-b_{21}-b_{22} \\ h^2: & \frac{1}{2}-\frac{1}{2}b_{21}-b_{22}+\delta d_{21}-d_{21}-d_{22} \\ h^3: & \frac{1}{6}-\frac{1}{8}b_{21}-\frac{1}{2}b_{22}-\frac{1}{2}d_{21}-d_{22} \\ h^4: & \frac{1}{24}-\frac{1}{48}b_{21}-\frac{1}{6}b_{22}-\frac{1}{8}d_{21}-\frac{1}{2}d_{22} \end{array}\right\} \tag{10}$$

Combining the systems (9) and (10), the constants C_j are expressed in terms of the matrix coefficients as:

$$C_0: \begin{pmatrix}1\\1\end{pmatrix}-\begin{pmatrix}1\\1\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}$$

$$C_1: \begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^1-\begin{pmatrix}0&-\gamma b_{11}\\0&-\gamma b_{21}\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix}-\begin{pmatrix}b_{11}&b_{12}\\b_{21}&b_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^0$$

$$C_2: \begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^2-2\begin{pmatrix}b_{11}&b_{12}\\b_{21}&b_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^1-2\begin{pmatrix}0&-\delta d_{11}\\0&-\delta d_{21}\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix}-2\begin{pmatrix}d_{11}&d_{12}\\-\delta d_{22}&d_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^0$$

$$C_3: \begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^3-3\begin{pmatrix}b_{11}&b_{12}\\b_{21}&b_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^2-6\begin{pmatrix}d_{11}&d_{12}\\-\delta d_{22}&b_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^1$$

$$C_4: \begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^4-4\begin{pmatrix}b_{11}&b_{12}\\b_{21}&b_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^3-12\begin{pmatrix}d_{11}&d_{12}\\-\delta d_{22}&b_{22}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix}^2$$

Setting the system (9) equal to zero and solving simultaneously by the method of undetermined coefficients, the solution of the first component is obtained as:

$$b_{11}=-\frac{1+26\delta}{4(1+4\gamma-8\delta+16\gamma\delta)},\ b_{12}=-\frac{-3-7\gamma-10\delta-6\gamma\delta}{4(1+4\gamma-8\delta+16\gamma\delta)},\ d_{11}=-\frac{17+44\gamma}{48(1+4\gamma-8\delta+16\gamma\delta)},$$
$$d_{12}=-\frac{7+16\gamma+29\delta+20\gamma\delta}{48(1+4\gamma-8\delta+16\gamma\delta)}$$

Similarly, setting (10) equal to zero and solving yields

$$b_{21}=-\frac{8\delta}{1+4\gamma-8\delta+16\gamma\delta},\ b_{22}=-\frac{-1-4\gamma-8\gamma\delta}{1+4\gamma-8\delta+16\gamma\delta},\ d_{21}=-\frac{1+4\gamma}{3(1+4\gamma-8\delta+16\gamma\delta)},$$
$$d_{22}=-\frac{1+4\gamma+2\delta+8\gamma\delta}{6(1+4\gamma-8\delta+16\gamma\delta)}$$

By evaluating the solutions at $\gamma=\delta=-\frac{1}{5}$, the coefficients are generated and the schemes in the two-point block method are given as:

$$-y_n+y_{n+\frac{1}{2}}=\frac{21}{244}h\,f_n+\frac{105}{244}h\,f_{n+\frac{1}{2}}-\frac{1}{61}h\,f_{n+1}-\frac{41}{2928}h^2\,f'_n-\frac{205}{2928}h^2\,f'_{n+\frac{1}{2}}+\frac{5}{488}h^2\,f'_{n+1}$$
$$-y_n+y_{n+1}=\frac{8}{61}h\,f_n+\frac{40}{61}h\,f_{n+\frac{1}{2}}+\frac{13}{61}h\,f_{n+1}-\frac{1}{183}h^2\,f'_n-\frac{5}{183}h^2\,f'_{n+\frac{1}{2}}-\frac{1}{122}h^2\,f'_{n+1}$$

2.2 Coefficients of proposed methods

Since I_k and A_1 are predetermined from the structure of the proposed method (5), the coefficients B_1, B_0, D_1 and D_0 of the proposed method are given.

Two-point block method

$$B_1=\begin{pmatrix}0 & \frac{21}{244}\\ 0 & \frac{8}{61}\end{pmatrix},B_0=\begin{pmatrix}\frac{105}{244} & -\frac{1}{61}\\ \frac{40}{61} & \frac{13}{61}\end{pmatrix},\ D_1=\begin{pmatrix}0 & -\frac{41}{2928}\\ 0 & -\frac{1}{183}\end{pmatrix},\quad D_0=\begin{pmatrix}-\frac{205}{2928} & \frac{5}{488}\\ -\frac{5}{183} & -\frac{1}{122}\end{pmatrix}$$

Three-point block method

$$B_1=\begin{pmatrix}0 & 0 & \frac{2197}{24480}\\ 0 & 0 & \frac{343}{3060}\\ 0 & 0 & \frac{309}{2720}\end{pmatrix},\ B_0=\begin{pmatrix}\frac{2197}{4896} & -\frac{661}{24480} & -\frac{4361}{24480}\\ \frac{343}{612} & \frac{401}{3060} & -\frac{419}{3060}\\ \frac{309}{544} & \frac{843}{2720} & \frac{23}{2720}\end{pmatrix},\ D_1=\begin{pmatrix}0 & 0 & -\frac{13}{14688}\\ 0 & 0 & \frac{1}{612}\\ 0 & 0 & \frac{1}{544}\end{pmatrix},$$

$$D_0=\begin{pmatrix} -\frac{65}{14688} & \frac{2177}{24480} & \frac{151}{8160} \\ \frac{5}{612} & \frac{559}{9180} & \frac{131}{9180} \\ \frac{5}{544} & \frac{209}{2720} & \frac{21}{2720} \end{pmatrix}$$

Four-point block method

$$B_1=\begin{pmatrix} 0 & 0 & 0 & \frac{2040583}{23296896} \\ 0 & 0 & 0 & \frac{18031}{182007} \\ 0 & 0 & 0 & \frac{85669}{862848} \\ 0 & 0 & 0 & \frac{18128}{182007} \end{pmatrix}, B_0=\begin{pmatrix} \frac{10202915}{23296896} & \frac{344429}{862848} & -\frac{1773781}{3328128} & -\frac{235885}{1664064} \\ \frac{90155}{182007} & \frac{10931}{26964} & -\frac{10321}{26001} & -\frac{10697}{104004} \\ \frac{428345}{862848} & \frac{50181}{95872} & -\frac{33391}{123264} & -\frac{6055}{61632} \\ \frac{90640}{182007} & \frac{3712}{6741} & -\frac{3824}{26001} & -\frac{31}{26001} \end{pmatrix},$$

$$D_1=\begin{pmatrix} 0 & 0 & 0 & \frac{248257}{155312640} \\ 0 & 0 & 0 & \frac{1499}{606690} \\ 0 & 0 & 0 & \frac{14323}{5752320} \\ 0 & 0 & 0 & \frac{764}{303345} \end{pmatrix}, D_0=\begin{pmatrix} \frac{248257}{31062528} & \frac{805969}{5752320} & \frac{16281901}{155312640} & \frac{707857}{77656320} \\ \frac{1499}{121338} & \frac{18079}{179760} & \frac{23371}{303345} & \frac{31979}{4853520} \\ \frac{14323}{1150464} & \frac{202779}{1917440} & \frac{401719}{5752320} & \frac{18163}{2876160} \\ \frac{764}{60669} & \frac{1223}{11235} & \frac{25532}{303345} & \frac{2141}{606690} \end{pmatrix}$$

Five-point block method

$$B_1=\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{7425533}{95256000} \\ 0 & 0 & 0 & 0 & \frac{4015679}{47628000} \\ 0 & 0 & 0 & 0 & \frac{19843}{235200} \\ 0 & 0 & 0 & 0 & \frac{125606}{1488375} \\ 0 & 0 & 0 & 0 & \frac{64385}{762048} \end{pmatrix}, B_0=\begin{pmatrix} \frac{7425533}{19051200} & \frac{1158923}{1270080} & -\frac{289411}{762048} & -\frac{979033}{1360800} & -\frac{1285423}{15876000} \\ \frac{4015679}{9525600} & \frac{138793}{198450} & -\frac{175531}{595350} & -\frac{627653}{1360800} & -\frac{780953}{15876000} \\ \frac{19843}{47040} & \frac{61543}{78400} & -\frac{45691}{235200} & -\frac{377}{840} & -\frac{943}{19600} \\ \frac{125606}{297675} & \frac{78544}{99225} & -\frac{28048}{297675} & -\frac{15182}{42525} & -\frac{23162}{496125} \\ \frac{321925}{762048} & \frac{205775}{254016} & -\frac{44675}{762048} & -\frac{15425}{54432} & \frac{3173}{127008} \end{pmatrix},$$

$$D_1=\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{507413}{317520000} \\ 0 & 0 & 0 & 0 & \frac{15487}{7938000} \\ 0 & 0 & 0 & 0 & \frac{7661}{3920000} \\ 0 & 0 & 0 & 0 & \frac{4852}{2480625} \\ 0 & 0 & 0 & 0 & \frac{997}{508032} \end{pmatrix}, D_0=\begin{pmatrix} \frac{507413}{63504000} & \frac{781357}{5292000} & \frac{512131}{2268000} & \frac{4744199}{63504000} & \frac{391709}{105840000} \\ \frac{15487}{1587600} & \frac{66961}{661500} & \frac{42253}{283500} & \frac{371591}{7938000} & \frac{1181}{529200} \\ \frac{7661}{784000} & \frac{20319}{196000} & \frac{3979}{28000} & \frac{35807}{784000} & \frac{8559}{3920000} \\ \frac{4852}{496125} & \frac{17216}{165375} & \frac{10448}{70875} & \frac{21052}{496125} & \frac{1756}{826875} \\ \frac{4985}{508032} & \frac{4465}{42336} & \frac{2815}{18144} & \frac{28115}{508032} & \frac{109}{169344} \end{pmatrix},$$

3. Order, Error Constants and Stability of Proposed Method

The properties of the proposed method (5) are presented in this section. The order condition is given as:

Let $e=(1,1,\cdots,1)^T$ and $c=(v_1,v_1,\cdots,1)^T$.

$$C_0=e-A_1e$$

$$C_1=c^1-B_1e-B_0e$$

$$C_2=c^2-2B_0c^1-2D_1e-2D_0c^0$$

$$C_3=c^3-3B_0c^2-6D_0c^1$$

$$C_4=c^4-4B_0c^3-12D_0c^2$$

$$\vdots$$

$$C_j=c^j-j\,B_0c^{j-1}-j(j-1)D_0c^{j-2},\qquad j=5,6,\cdots$$

The powers of the vectors in C_j are component-wise. The *k*-point block method (5) is of order p if $C_j=0$ for $j=0,1,\cdots,p$ and $C_{p+1}\neq 0$.

Lemma

The proposed method is of order *p* = 2k.

Proof

Suppose that Z_m is the exact solution to (1), then the local truncation error E_m is given as

$$\begin{aligned} E_m &= Z_m-I_kY_m-A_1Y_{m-1}+\gamma hB_1F(Y_{m-1})-hB_0F(Y_m)+\delta h^2D_1F'(Y_{m-1})-h^2D_0F'(Y_m) \\ &= C_{p+1}h^{2k+1}Y^{(2k+1)}(t)+\mathrm{O}(h^{2k+2}) \end{aligned}$$

where $C_{p+1}h^{2k+1}Y^{(2k+1)}(t)$ is the principal truncation error.

For Two-point block method (5), the local truncation error for each constituent scheme with values of γ and δ given as $-\frac{1}{5}$ is $\left(-\frac{599}{1405440}h^5y^{(5)}(t)+O(h^6),\ -\frac{7}{21960}h^5y^{(5)}(t)+O(h^6)\right)^T$, the error constant is $C_5=\left(-\frac{599}{1405440},-\frac{7}{21960}\right)^T$ and order is $p=(4,4)^T$. □

The error constants of the proposed method for $2\le k\le 5$ are presented in Table 1.

Table 1: Order and error constants of proposed method

k	Order	Error constants
2	4	$\left(-\frac{599}{1405440},-\frac{7}{21960}\right)^T$
3	6	$\left(-\frac{19049}{11242929600},-\frac{1}{351341550},-\frac{491}{416404800}\right)^T$
4	8	$\left(-\frac{1545809}{712499842252800},-\frac{32399}{22265620070400},-\frac{37411}{2638883046400},-\frac{929}{695800627200}\right)^T$
5	10	$\left(-\frac{24102223}{1719073125000000000},-\frac{2269}{3357564697265625},-\frac{140191}{2122312500000000000},-\frac{10909}{16787823486328125},\frac{16319}{275051700000000000}\right)^T$

The zero-stability of proposed method (5) is examined as:

$$\det\left(I_k w - A_1\right) = 0$$

$$w^{k-1}(w-1) = 0$$

The roots $w_k = 1, w_{k-1} = w_{k-2} = \cdots = w_2 = w_1 = 0$ of the first characteristic polynomial (5) are all less than 1 and the principal root is simple. Thus, the block method (5) is zero-stable.

Applying (5) to the test equations $y' = -\lambda y$ and $y'' = -\lambda^2 y$, it yields the stability polynomial

$$\pi(w,z) = \det(I_k w - A_1 + z\,\gamma\, B_1 - zB_0 w + z^2\,\delta\, D_1 - z^2 D_0 w) = 0\,. \tag{11}$$

The plots of the stability domain employed the technique of boundary locus [3]. This was done using codes in MATHEMATICA 13.2 (Wolfram Research, Illinois, USA) on a 64-bit computer. The stability regions for the proposed method are presented in Figure 1. The unbounded regions in the figures indicate the region of absolute stability of (5).

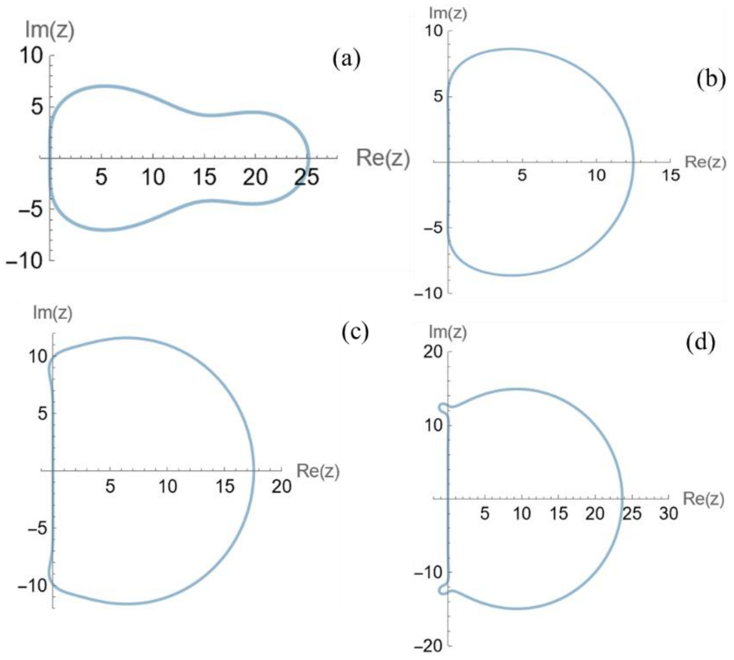

Figure 1: Stability plots for (a) two-point, (b) three-point, (c) four-point, and (d) five-point methods

3. Implementation and Numerical Results

The implementation of the proposed method (5) to integrate a system of stiff initial value problem (1) results into an algebraic system of the form:

$$A_0 Y_m = hB_0 F(Y_m) + h^2 D_0 F'(Y_m) + \chi_{m-1}, \tag{12}$$

where $\chi_{m-1} = A_1 Y_{m-1} - \gamma\, hB_1 F(Y_{m-1}) - \delta\, h^2 D_1 F'(Y_{m-1})$ is a known function of previously computed set of values. Set $F(Y_m)$ as

$$F(Y_m) = A_0 Y_m - hB_0 F(Y_m) + h^2 D_0 F'(Y_m) + \chi_{m-1}\,. \tag{13}$$

The system (13) is solved for the vector Y_m using fixed point iteration or by some form of Newton's method [11]. The implicitness of the method is resolved by using a modified Newton-Raphson technique [11]. This technique approximates the Jacobian, thereby reducing the cost of the computation. All computations were carried out with MATLAB version R2021b (MathWorks Inc., Massachusetts, USA) using a 64-bit computer.

The Newton iteration takes the form

$$J(Y_m^{[r+1]} - Y_m^{[r]}) = -F(Y_m^{[r]}) \tag{14}$$

where $r = 0,1,\cdots$ and J is the Jacobian matrix.

Numerical results generated by the proposed method (5) are compared to numerical solutions generated by the following methods in the literature:

i. Generalized Cash-type second derivative extended backward differentiation formulas (GCE2BD) [13];

ii. Multi-derivative multistep method (MDMM) [14];

iii. Order six block integrators (OSBI) [15];

iv. Extended continuous block backward differentiation formula (ECBBDF) [16]; and

v. Second derivative extended backward differentiation formulae (E2BD) [17].

The following test problems are considered for the comparison of numerical experiments.

Test Problem 1
Consider the initial value problem

$$y' = \mu(1-y), \quad y(o) = \frac{1}{2}, \qquad \mu = \frac{1}{2}.$$

Its exact solution is given as $y(t) = 1 - \mu e^{-\mu t}$, [14].

Test Problem 2
Consider the problem

$$y_1' = -2000y_1 + 1000y_2 + 1, \qquad y_1(0) = 0$$
$$y_2' = y_1 - y_2, \qquad y_2(0) = 0$$

with exact solutions $y_1(t) = -0.000497e^{-2000.5t} - 0.0005034e^{-0.5t} + 0.001$ and $y_2(t) = -0.00000025e^{-2000.5t} - 0.001007e^{-0.5t} + 0.001$, [13], [16].

Test Problem 3

Consider the initial value problem

$$y_1' = -\alpha y_1 - \beta y_2 + (\alpha + \beta - 1)e^{-t}, \qquad y_1(0) = 1$$

$$y_2' = \beta y_1 - \alpha y_2 + (\alpha - \beta - 1)e^{-t}, \qquad y_2(0) = 1$$

with exact solutions are $y_1(t) = y_2(t) = e^{-t}$ and $y_3(t) = t$, [17].

The numerical results of the experiment for Test Problem 1 to 3 are displayed in Table 2 to Table 4 along with methods in the literature. The solution plots are shown in Figures 2 to 4.

Table 2: Absolute error $\| y_i(t) - y_{ih} \|$ for Test Problem 1

	OSBI	MDMM	Proposed Method (5)
t	p = 6	p = 6	p = 5
0.1	2.0×10^{-11}	3.766×10^{-12}	4.440×10^{-16}
0.2	3.0×10^{-11}	2.498×10^{-12}	7.771×10^{-16}
0.3	1.0×10^{-10}	3.013×10^{-12}	1.110×10^{-15}
0.4	2.0×10^{-10}	2.408×10^{-12}	1.332×10^{-15}
0.5	1.0×10^{-10}	5.374×10^{-12}	1.665×10^{-15}
0.6	2.0×10^{-10}	4.225×10^{-12}	1.887×10^{-15}
0.7	1.0×10^{-10}	4.538×10^{-12}	2.109×10^{-15}
0.8	2.0×10^{-10}	3.943×10^{-12}	2.331×10^{-15}
0.9	3.0×10^{-10}	6.274×10^{-12}	2.442×10^{-15}
1.0	3.0×10^{-10}	5.242×10^{-12}	2.664×10^{-15}

Table 3: Absolute error $\| y_i(t) - y_{ih} \|$ for Test Problem 2

h	*t*	y_i	ECBBDF p = 8	GCE2BD p = 8	Proposed Method (5) p = 8
0.0001	5	y_1	2.328953×10^{-7}	2.328953×10^{-7}	2.328953×10^{-7}
		y_2	5.027468×10^{-7}	5.027468×10^{-7}	5.027468×10^{-7}
	10	y_1	1.700858×10^{-8}	1.699965×10^{-8}	1.700768×10^{-8}
		y_2	3.705176×10^{-8}	3.703239×10^{-8}	3.704982×10^{-8}
0.1	5	y_1	3.163426×10^{-4}	2.328953×10^{-7}	2.210483×10^{-7}
		y_2	6.610743×10^{-7}	5.027469×10^{-7}	4.772507×10^{-7}
	10	y_1	2.005234×10^{-4}	1.700858×10^{-8}	1.613892×10^{-8}
		y_2	1.373470×10^{-7}	3.705176×10^{-8}	3.516448×10^{-8}

Table 4: Absolute error $\| y_i(t) - y_{ih} \|$ for Test Problem 3

t	y_i	E2BD Class 1 $p = 8$	E2BD Class 2 $p = 8$	GCE2BD p = 8	Proposed method (5) p = 8
4.5	y_1	0.1×10^{-10}	0.1×10^{-10}	0.6×10^{-14}	0.4×10^{-16}
	y_2	0.1×10^{-10}	0.1×10^{-10}	0.8×10^{-15}	0.1×10^{-16}
9.0	y_1	0.1×10^{-12}	0.1×10^{-12}	0.3×10^{-16}	0.1×10^{-18}
	y_2	0.1×10^{-12}	0.1×10^{-12}	0.1×10^{-16}	0.8×10^{-19}
13.5	y_1	0.1×10^{-15}	0.1×10^{-11}	0.8×10^{-18}	0.4×10^{-20}
	y_2	0.1×10^{-15}	0.1×10^{-11}	0.5×10^{-18}	0.2×10^{-21}
18.0	y_1	0.1×10^{-17}	0.1×10^{-11}	0.1×10^{-19}	0.6×10^{-22}
	y_2	0.1×10^{-17}	0.1×10^{-11}	0.2×10^{-20}	0.1×10^{-22}

3.1 Discussion of Results

The proposed Off-node block method of order 6 was applied to Test Problem 1 and the error computed over the interval $0 \le t \le 1$. The results were compared to the OSBI [15] and MDMM [14] of the same order using $h = 0.1$. The results in Table 2 revealed that the proposed method outperformed the OSBI and MDMM methods. The solution plots of the proposed method versus the exact solution are presented in Figure 2.

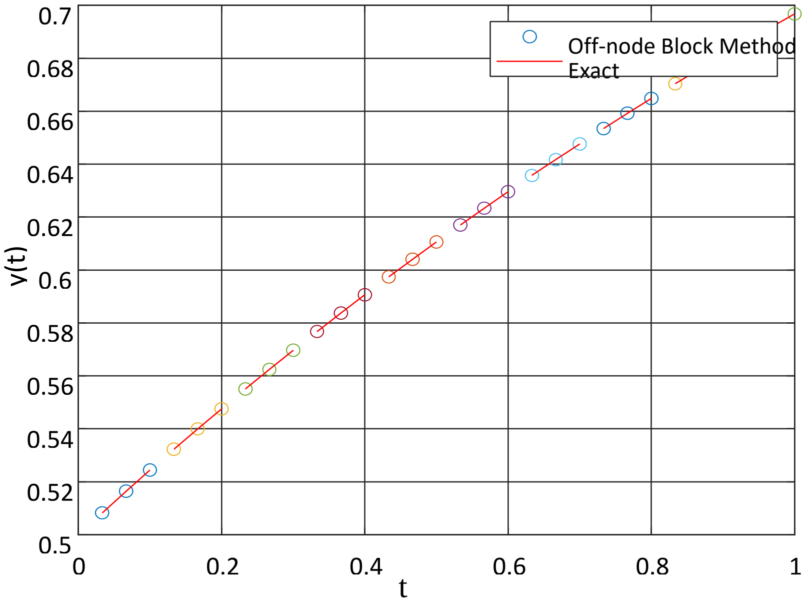

Figure 2: Solution plot of Test Problem 1 h = 0.1 and t = 1

The proposed method of order 8 was used to integrate Test Problem 2 at points $t = 5$ and $t = 10$ using step sizes $h = 0.0001$ and $h = 0.1$. The results of the absolute error in Table 3 were compared to the ECBBDF [16] and the GCE2BD method [13]. Results in Table 3 indicate that the proposed method showed comparable accuracy to the ECBBDF and GCE2BD methods when the step size is smaller but outperformed the methods for larger step size $h = 0.1$. From the solution plot of approximate and exact solutions in Figure 3, it is observed that the proposed method mimics the exact solution trajectory.

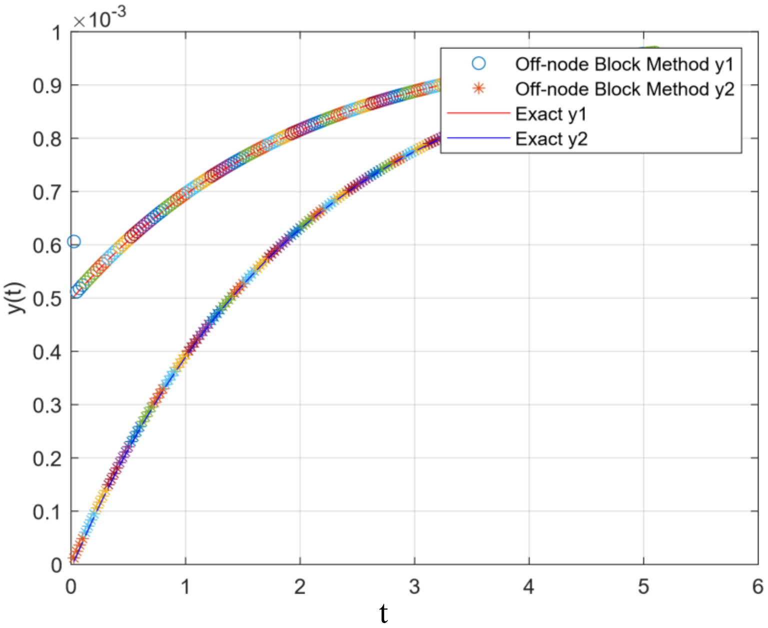

Figure 3: Solution plot of proposed method for Test Problem 2, $h = 0.1$, $t = 5$

The proposed method of order 8 was used to integrate Test Problem 3 at different points using step size $h = 0.09$. The results were compared to the GCE2BD method [13] and the E2BD methods of class 1 and class 2 in Ref. [17]. The proposed method showed superior accuracy to the methods in comparison. The numerical results of the solution components are shown in Table 4, indicating that the proposed method consistently yields smaller errors than GCE2BD and E2BD methods. The solution plot in Figure 4 illustrates how closely the solution of the proposed method follows the exact solution trajectories.

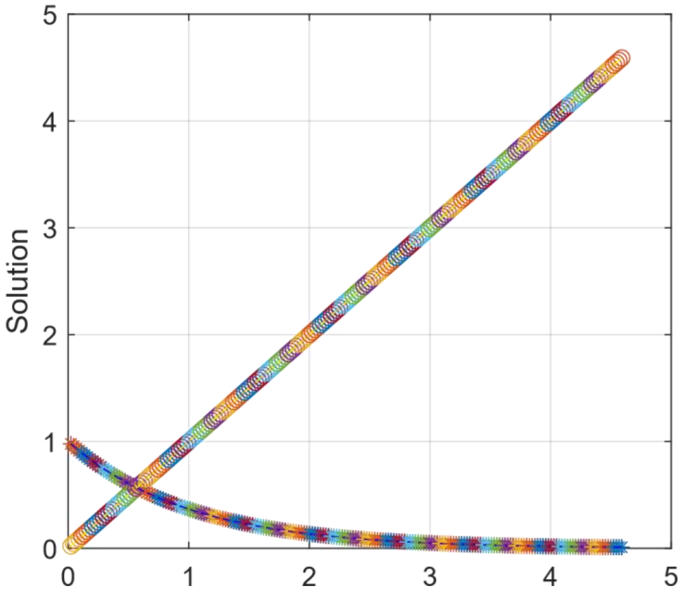

Figure 4: Solution Plot of proposed method for Test Problem 3, $h = 0.09$, $t = 4.5$

4. Conclusion

The challenges associated with solving stiff Initial Value Problems were highlighted. A class of off-node block methods was developed for the integration of stiff IVPs in ODEs. The methods were constructed via Taylor's series expansion. The basic properties of the methods were examined. Numerical experiments were performed on standard test problems and were compared to those of existing methods in the literature. Numerical results generated from the proposed method showed superiority in terms of accuracy to existing methods in the literature.

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Conflict of interests
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Conceptualisation, U.P.A.; methodology, U.P.A. and K.O.M.; software, U.P.A.; validation, K.O.M; formal analysis, U.P.A. investigation, U.P.A. and K.O.M; resources, U.P.A. and K.O.M.; writing—original draft preparation, U.P.A.; writing—review and editing, U.P.A and K.O.M.; visualisation, U.P.A.; supervision, K.O.M. All authors have read and agreed to the published version of the manuscript

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