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Third Derivative Block Methods for Stiff Initial Value Problems

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Abstract:
In this paper, we developed a continuous third derivative block method using polynomial approximate solution for the solution of stiff first order initial value problems of ordinary differential equations. The development of the technique involved the interpolation and collocation of the polynomial approximate solution which give a Continuous Linear Multistep Method (CLMM). The CLMM is evaluated at some selected grid points to give discrete methods which are implemented in block form. Two cases among others are implemented, the methods are convergent and L-stable. Numerical results show that the methods are effective and computationally reliable for stiff problems.
Key Word*: Stiff ODEs, Block Method, Third Derivative, interpolation and collocation, Stability.*

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I. Introduction

In this work, we focused on the numerical integration of first order stiff initial value problems (IVPs) of the form

$$y' = f(x, y(x)), y(x_n) = y_0, x \in [x_n, x_N] \quad (1)$$

Where $f: [x_n, x_N] \times \mathbb{R}^m \to \mathbb{R}^m, y_0 \epsilon \mathbb{R}^m$ is continuously differentiable, moreover, the Jacobian (J) arising from (1) varies slowly and the eigenvalues of J have negative real parts. The desire to develop methods that will integrate (1) and also, control its special properties (Stiffness, Oscillatory, etc.) has drawn much attention of scholars, among them are [1, 2,3,4]. Stiffness is a subtle, difficult and important concept in the numerical solution of ODEs, it depends on the DEs, the initial condition and the interval under consideration [5]. It is a well-known fact that (1) always occur in engineering and control systems. [6] noted that mathematical formulation of new models of physical situations in engineering and sciences often lead to systems of the form (1) and as such, there is a need to generate techniques to conveniently cope with these types of problems. The search for better methods for solving these stiff systems leads to the discovery of the Backward Differentiation Formulae (BDF) [7, 8], since then, most of the improvements in the class of linear multistep methods have been based on the BDF, because of its special properties.

[9] worked on the hybrid BDF with one additional off-grid point introduced in the first derivative of the solution to improve the absolute stability region of the method. [10] noted that the search for higher order A-stable multistep methods is carried out in two main directions: the use of higher derivatives of the solutions and the use additional stages, off-step points, super-future points. We are therefore motivated with the point raised by [10] to consider higher derivative method to construct LMM for the solution of first order stiff (IVPs).

Assumption 1.1. In ODEs (1), the function f belongs to $\mathbb{C}^1$-class and therefore satisfies the Lipschitz condition with the constant L . That is, if the estimation

$$\| f(x,y) - f(x,y^*) \| \leq \boldsymbol{L} \| \boldsymbol{y} - y^* \|$$

holds, L is called Lipschitz constant [2].

Theorem 1.1. If f satisfies Lipschitz condition with constant L then the initial value problem

$$y' = f(x, y(x)), y(x_n) = y_0$$

possesses a unique solution on the interval $[x_0, T]$ [1].

II. Mathematical procedures

We derive third derivative CLMM using polynomial approximate solution of the form

$$y(x)=\sum_{j=0}^{p} a_j x^j \quad (2)$$

where $a_j's$ are parameters to be determined. First, second and third derivative of (2) give

$$y'(x)=\sum_{j=1}^{p} j a_j x^{j-1} \qquad (3)$$

$$y''(x)=\sum_{j=2}^{p} j(j-1) a_j x^{j-2} \qquad (4)$$

$$y'''(x)=\sum_{j=3}^{p} j(j-2) a_j x^{j-3} \qquad (5)$$

Interpolating (2) at the point x_{n+i} and collocating (3), (4) and (5) at the point x_{n+i}, we therefore imposed the following conditions

$$y(x_{n+i})=y_{n+i}, i=0,1,\dots,r$$

$$y'(x_{n+i})=f_{n+i}, i=0,1,\dots,\lambda$$

$$y''(x_{n+i})=g_{n+i}, i=0,1,\dots,\kappa$$

$$y'''(x_{n+i})=l_{n+i}, i=0,1,\dots,\tau$$

Give a system of non-linear equations of the form

$$\boldsymbol{XA}=\boldsymbol{U} \quad (6)$$

Where;

$A=[a_0 \quad \cdots \quad a_p\ ]^T, for\ p=r+\lambda+\kappa+\tau+1$

$$U=[y_n \quad \cdots \quad y_{n+r} f_n \quad \dots \quad f_{n+\lambda} g_n \quad \cdots \quad g_{n+\kappa} l_n \quad \dots \quad l_{n+\tau}]^T$$

$$X = \begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 & & x_n^m \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & x_{n+1}^4 & x_{n+1}^5 & \cdots & x_{n+1}^m \\ & & \vdots & & & & \ddots & \vdots \\ 1 & x_{n+r} & x_{n+r}^2 & x_{n+r}^3 & x_{n+r}^4 & x_{n+r}^5 & & x_{n+r}^m \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & 5x_n^4 & & mx_n^{m-1} \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 4x_{n+1}^3 & 5x_{n+1}^4 & \cdots & mx_{n+1}^{m-1} \\ & & \vdots & & & & \ddots & \vdots \\ 0 & 1 & 2x_{n+\lambda} & 3x_{n+\lambda}^2 & 4x_{n+\lambda}^3 & 5x_{n+\lambda}^4 & \cdots & mx_{n+\lambda}^{m-1} \\ 0 & 0 & 2 & 6x_n & 12x_n^2 & 20x_n^3 & & m(m-1)x_n^{m-2} \\ 0 & 0 & 2 & 6x_{n+1} & 12x_{n+1}^2 & 20x_{n+1}^3 & \cdots & m(m-1)x_{n+1}^{m-2} \\ & & \vdots & & & & \ddots & \vdots \\ 0 & 0 & 2 & 6x_{n+\kappa} & 12x_{n+\kappa}^2 & 20x_{n+\kappa}^3 & \cdots & m(m-1)x_{n+\kappa}^{m-2} \\ 0 & 0 & 0 & 6 & 24x_n & 60x_n^2 & & m(m-1)(m-2)x_n^{m-3} \\ 0 & 0 & 0 & 6 & 24x_{n+1} & 60x_{n+1}^2 & \cdots & m(m-1)(m-2)x_{n+1}^{m-3} \\ & & \vdots & & & & \ddots & \vdots \\ 0 & 0 & 0 & 6 & 24x_{n+\tau} & 60x_{n+\tau}^2 & \cdots & m(m-1)(m-2)x_{n+\tau}^{m-3} \end{bmatrix}$$

Solving (6) using Crammer's rule for the unknown parameters, substituting the result into (2) and after some algebraic sorting give third derivative CLMM in the form

$$y_{n+t} = \alpha_0(t)\, y_n + \sum_{i=1}^{3} h^i \sum_{j=0}^{k} \beta_j^i(t)\, f_{n+j}^{(i-1)} \tag{7}$$

2.1 Specification of the Method

The parameters of the third derivative method can be obtain by considering the CLMM (7), we set $t = \frac{x-x_n}{h}$ and introduce some points u, v to specified the method. These points are carefully chosen to guaranty the convergent of the block third derivative methods. Expanding (7) we have the following continuous scheme specified as

$$y_{t+1} = \alpha_0 y_n + h\left(\beta_0^1 f_n + \beta_u^1 f_{n+u} + \beta_v^1 f_{n+v}\right) + h^2 \beta_v^2 g_{n+v} + h^3 \beta_v^3 l_{n+v} \tag{8}$$

Where;

$$\beta_0^1 = \frac{1}{20}\frac{t}{uv^3}\left(4t^4 - 15t^3 v - 5ut^3 + 20t^2v^2 + 20ut^2 v - 10tv^3 - 30utv^2 + 20uv^3\right)$$

$$\alpha_0 = 1,\ \ \beta_u^1 = \frac{1}{20}\frac{t^2}{u(u-v)^3}\left(4t^3 - 15t^2 v + 20tv^2 - 10v^3\right)$$

$$\beta_v^1 = -\frac{1}{20}\frac{t^2}{v^3(u-v)^3}\begin{pmatrix}4t^3u^2 - 12t^3uv + 12t^3v^2 - 5t^2u^3 + 30t^2uv^2 - 40t^2v^3 + 20tu^3v \\ -40tu^2v^2 + 40tv^4 - 30u^3v^2 + 80u^2v^3 - 60uv^4\end{pmatrix}$$

$$\beta_v^2 = -\frac{1}{20}\frac{t^2}{v^2(u-v)^2}\begin{pmatrix}-4t^3u + 8t^3v + 5t^2u^2 + 5t^2uv - 25t^2v^2 \\ -20tu^2v + 20tuv^2 + 20tv^3 + 20u^2v^2 - 30uv^3\end{pmatrix}$$

$$\beta_v^3 = -\frac{1}{20}\frac{t^2}{v(u-v)^2}\left(12t^3 - 30t^2v - 15t^2u + 20tv^2 + 40utv - 30uv^2\right)$$

Evaluating (8) at $t = u, v$ and implementing in a block method give the following class of DLMMs as

$$A^{(1)}Y_m = A^{(0)}Y_{m-1} + hB^{(0)}F_{m-1} + hB^{(1)}F_m + h^2C^{(1)}G_m + h^3D^{(1)}L_m \qquad (9)$$

$$A^{(1)} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, A^{(0)} = \begin{bmatrix}0 & \alpha_{0u}\\ 0 & \alpha_{0v}\end{bmatrix}, B^{(0)} = \begin{bmatrix}0 & \beta^1{}_{0u}\\ 0 & \beta^1{}_{0v}\end{bmatrix},$$

$$B^{(1)} = \begin{bmatrix}\beta^1{}_{uu} & \beta^1{}_{vu}\\ \beta^1{}_{uv} & \beta^1{}_{uv}\end{bmatrix}, C^{(1)} = \begin{bmatrix}0 & \beta^2{}_{vu}\\ 0 & \beta^2{}_{vv}\end{bmatrix}, D^{(1)} = \begin{bmatrix}0 & \beta^3{}_{vu}\\ 0 & \beta^3{}_{vv}\end{bmatrix}$$

$$\alpha_{0u} = 1, \alpha_{0v} = 1, \beta^1{}_{0u} = \left(-\frac{u^4 - 5u^3v + 10u^2v^2 - 10uv^3}{20v^3}\right),$$

$$\beta^1{}_{0v} = -\frac{1}{20u}\left(v^2 - 5uv\right), \beta^1{}_{uu} = \frac{\left(4u^4 - 15u^3v + 20u^2v^2 - 10uv^3\right)}{\left(20u^3 - 60u^2v + 60uv^2 - 20v^3\right)},$$

$$\beta^1{}_{vu} = -\frac{\left(u^7 - 8u^6v + 28u^5v^2 - 40u^4v^3 + 20u^3v^4\right)}{\left(-20u^3v^3 + 60u^2v^4 - 60uv^5 + 20v^6\right)},$$

$$\beta^1{}_{uv} = -\frac{\left(v^5\right)}{\left(-20u^4 - 60u^3v + 60u^2v^2 - 20uv^3\right)}, \beta^1{}_{vv} = -\frac{\left(-15u^3v + 44u^2v^2 - 42uv^3 + 12v^4\right)}{\left(20u^3 - 60u^2v + 60uv^2 - 20v^3\right)}$$

$$\beta^2{}_{vv} = -\frac{1}{20(u-v)^2}\left(5u^2v^2 - 9uv^3 + 3v^4\right), \beta^2{}_{vu} = -\frac{\left(-u^6 - 7u^5v + 15u^4v^2 - 10u^3v^3\right)}{\left(20u^2v^2 - 40uv^3 + 20v^4\right)}$$

$$\beta^3{}_{vu} = -v^3\frac{\left(2v - 5u\right)}{\left(120u - 120v\right)}, \beta^3{}_{vu} = -\frac{\left(3u^5 - 10u^4v + 10u^3v^2\right)}{\left(120v^2 - 120uv\right)}$$

III. Analysis of the block methods

3.1 order of the block method

Let's apply linear operator $L\left[y(x);h\right]$ to (9) then

$$L\left[y(x);h\right]=A^{(1)}Y_m-A^{(0)}Y_{m-1}-hB^{(0)}F_{m-1}-hB^{(1)}F_m-h^2C^{(1)}G_m-h^3D^{(1)}L_m=0 \quad (10)$$

expanding (10) in Taylor series and comparing the coefficient of h gives

$$C_0=\alpha_0+\alpha_1+...+\alpha_j, C_1=\alpha_1+2\alpha_2+...+j\alpha_j$$

$$C_2=\frac{1}{2}\left(\alpha_1+2^2\alpha_2+...+j^2\alpha_j\right)-\left(\beta_0+\beta_1+...+\beta_j\right)$$

$$\vdots$$

$$C_q=\frac{1}{q!}\left(\alpha_1+2^2\alpha_2+...+j^2\alpha_j\right)-\frac{1}{(q-2)}\left(\beta_0+\beta_1+...+\beta_j\right), q=3,4,\cdots$$

According to [11,12,13,14,15,16] (9) has order p if $C_0=C_1=\cdots=C_p=C_{p+1}\neq 0.C_{p+1}$ is the error constant

and $C_{p+1}h^{p+1}y^{p+1}(x_n)+0\left(h^{p+2}\right)$ is the truncation error at point x_n.

We have presented the order and the error constant of the third derivative block method in the table below.

Table 1: Order and Error Constant of the Third Derivative methods

Method	Order	Error Constant
y_{n+u}	4	$-\frac{1}{7200}u^3\left(2u^3-9u^2v+15uv^2-10v^3\right)$
y_{n+v}	4	$-\frac{1}{7200}v^5\left(v-3u\right)$

3.2 Consistency of the block method

(9) is said to be consistent if the order of the individual members is greater or equal to one, i.e., if $p\geq 1$ .The order of the block method is $p=(4,4)^T\geq 1$ hence it is consistent [12].

(9) is said to be zero stable if the roots $\lambda_s=1,2,...,n$ of the first characteristic polynomial $\rho(\lambda)$, defined by

$$\rho(\lambda)=\det\left[\lambda A^{(1)}-A^{(0)}\right]=0 \quad (11)$$

satisfies $|\lambda_s|\leq 1$ and every root with $|\lambda_s|=1$ has multiplicity not exceeding 1 in the limit as $h\to 0$.

$$\lambda = \{0,1\} \quad (12)$$

3.3 Convergence

Numerical method is said to be convergent if it is consistent and zero-stable [6]

3.4 Regions of Absolute Stability

3.4.1 *Linear Stability*

The linear-stability of block method is done by applying the block method to the test equations $y' = \lambda y$, where λ is supposed to run through the negative eigenvalues of the Jacobian matrix $\frac{\partial y}{\partial x}$. Letting $z = \lambda h$ it is easily shown that the application of method to the test equation yields

$$Y_\mu = M(z)Y_{\mu-1}, M(z) := \left[A^{(1)} - zB^{(1)} - z^2C^{(1)} - z^3D^{(1)}\right]^{-1}\left[A^{(0)} + z^2B^{(0)}\right] \quad (13)$$

where the matrix $M(z)$ is the amplification matrix which determines the stability function of the method.

$$M(z) = -6\frac{-20u + 4zu^2 - zu^2 + z^2v^2 - 5z^2uv - z^3uv^2 + z^3u^2v - 3zuv}{u\left(18z^2v^2 - 2z^3v^3 - 24zv - 72zv + 18z^2uv - 6z^3v^2u + z^4uv^3 + 120\right)} \quad (14)$$

As $z \to \infty$, $M(z)$=0, then we conclude that the method is $L - stable$

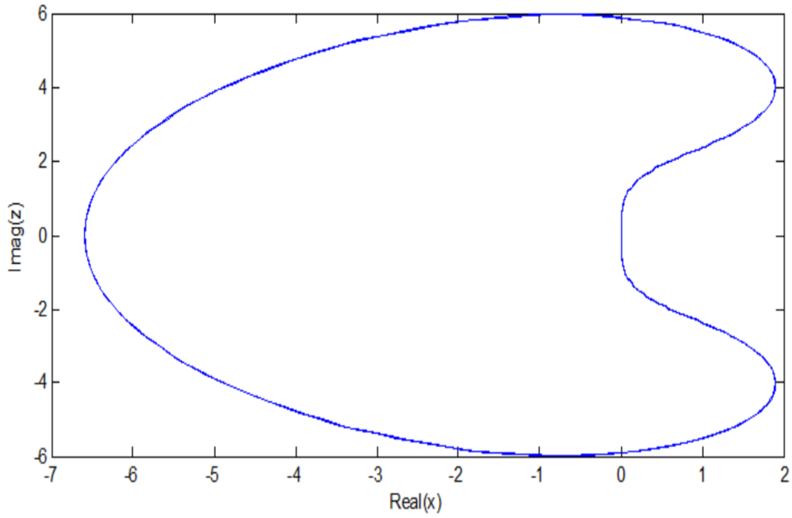

Fig.1. Region of Absolute Stability

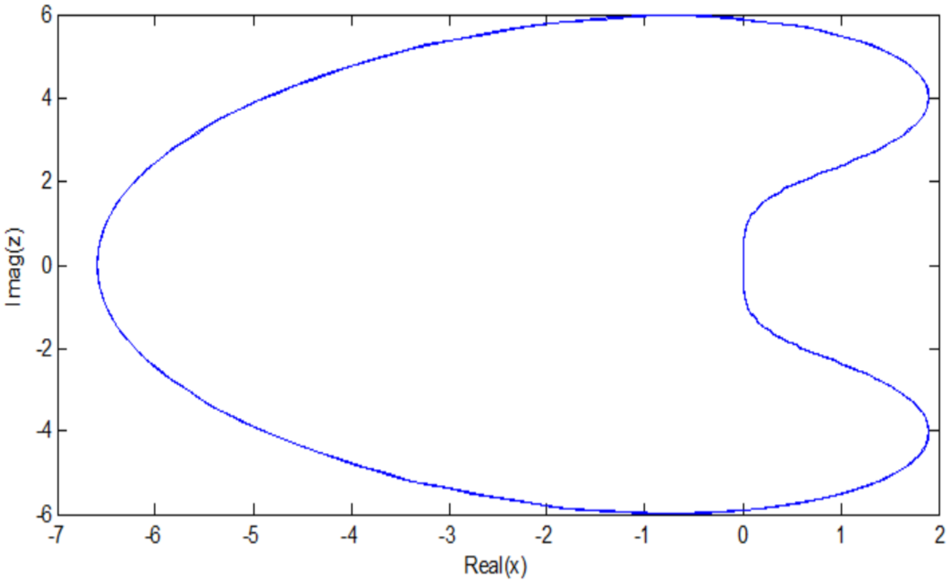

Fig.2. Region of Absolute Stability

In this paper, we consider two cases that belongs to the class of this method among others.

Case I: Weconsider two step method with equal intervals, that is, $u = 1, v = 2$

We obtained third derivative block method of order $[4 \quad 4]^T$, an error constant $\left[\frac{1}{200} \quad \frac{1}{255}\right]^T$ with region of absolute stability as shown in figure 1.

Case II: We consider one step hybrid method that is, $u = \frac{1}{2}, v = 1$

We obtained a class of hybrid third derivative block method of order $[4 \quad 4]^T$, with an error constant $\left[\frac{1}{12800} \quad \frac{1}{14400}\right]^T$ with region of absolute stability as shown in figure 2

IV. Numerical Examples

We consider the following linear and non-linear problems to test the efficiency of the developed methods. The following notation will be used in the presentation of the result.

$(3BEBDF)$ =3-Point Block Extended Backward Differentiation Formula of order five [16].

$(3BBDF)$ = 3-Point Block Backward Differentiation Formula [17].

abs = Absolute error

$abs(y - y_n) = y$ is the exact result and y_n is the computed result

Max = Maximum

h = Step-size

Example I:

$$\begin{bmatrix} y'_1(x) \\ y'_2(x) \end{bmatrix} = \begin{bmatrix} 9y_1 + 24y_2 + 5\cos x - \frac{1}{3}\sin x \\ -24y_1 - 51y_2 - 9\cos x + \frac{1}{3}\sin x \end{bmatrix}, \begin{bmatrix} y_1(0) = \frac{4}{3} \\ y_2(0) = \frac{2}{3} \end{bmatrix}$$

$$h = 0.01, 0 \le x \le 10 \text{ with the exact solution}$$

$$y_1(x) = 2e^{-3x} - e^{-39x} + \frac{1}{3}\cos x$$

$$y_1(x) = -e^{-3x} + 2e^{-39x} - \frac{1}{3}\cos x$$

Source :[16,17]

Table 2: Comparison of $Max(abs(y - y_n))$ for example I

h	$case\ I$	$case\ II$	$(3BEBDF)$	(3BBDF)
0.01	7.7631(-004)	8.4073(-005)	1.68449(-001)	6.62694(+099)
0.001	7.7631(-004)	9.3090(-006)	5.14997(-002)	7.44768(-002)
0.0001	7.5050(-005)	9.3089(-006)	6.95725(-003)	8.45376(-003)
0.00001	7.5030(-005)	1.5284(-006)	7.16727(-004)	8.53717(-004)

Example II:

$$y' = -100(y^2 - y), y(0) = 2, \ Exact\ y(x) = e^{-100x} + 1$$

$$h = 0.01, 0 \le x \le 10$$

Source :[16,17]

Table 3: Comparison of $Max(abs(y - y_n))$ for example II

h	$case\ I$	$case\ II$	$(3BEBDF)$	(3BBDF)
0.01	2.2204 (-016)	0	1.83156 (-002)	1.47562 (+128)
0.001	1.1102(-015)	1.1102(-15)	3.45336 (-002)	6.92223 (-002)
0.0001	1.1102(-014)	1.1102(-014)	8.42901 (-003)	1.07264 (-002)

Example III:

$$y' = \frac{50}{y} - 50y, y(0) = \sqrt{2}, \ Exact\ y(x) = \sqrt{e^{-100x} + 1}$$
$$h = 0.01, \ 0 \le x \le 1$$
$$Source : [16,17]$$

Table 4: Comparison of $Max(abs(y - y_n))$ for example III

h	$case\ I$	$case\ II$	$(3BEBDF)$	(3BBDF)
0.01	1.1102(-015)	1.1102(-015)	8.35838 (-003)	5.49256 (+009)
0.001	1.1102(-014)	1.1102(-014)	1.29425 (-002)	2.69497(-002)
0.0001	1.1102(-013)	1.1102(-013)	2.70535 (-003)	3.82432 (-003)

V. Conclusion

To crown it all, third derivative block methods for the solution of first order stiff IVPs of ODEs has been developed. Two cases among others are implemented using MATLAB8.5 Source code. The methods are convergent and L-stable. Numerical results show that the methods are effective and computationally reliable for stiff problems.

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