Stability analysis of third derivative multi-step methods for stiff initial value problems

Zohreh Eskandari
Department of Mathematics,
Shahrekord University, Shahrekord, Iran.
E-mail: zohre.eskandari.math.iut@gmail.com

Mohammad Shafi Dahaghin∗
Department of Mathematics,
Shahrekord University, Shahrekord, Iran.
E-mail: msh-dahaghin@sci.sku.ac.ir

Abstract
In this paper we present two class of third derivative multi-step methods (TDMMs) that have good stability properties. Stability analysis of these methods are examined and our numerical results are compared with the results of the existing method.

Keywords. Stiff ODEs, multi-step methods, Super-future point technique, Stability analysis.

1. Introduction

Many numerous work have focused on the development of more advanced and efficient methods for stiff problems [8, 11]. Enright, in [4] used the second derivative multi-step methods for stiff ordinary differential equations. Cash used extended backward differentiation formula for integration of stiff systems of ODEs and stiff initial value problems in ODEs and also used the second derivative extended backward differentiation formulas for the numerical integration of stiff systems [1, 2, 3]. Ibrahim and Ismail applied the new efficient second derivative multi-step methods for solving stiff systems [10]. Also, Hojjati, Hosseini and Rahimi Ardabili used the new second derivative multi-step methods for stiff systems [9]. Dahaghin and Eskandari surveyed stability analysis of the new second derivative multi-step method [7]. Ezzeddine introduced third derivative multi-step methods in [6] and a class of these methods was introduced in this paper. A potentially good numerical method for the solution of stiff systems of ODEs must have good accuracy and some reasonably wide region of absolute stability. A-stability requirement puts a sever limitation on the choice of suitable methods for stiff problems. The search for higher order A-stable multi-step methods is carried out in the two main directions. (a) Use higher derivatives of the solutions. (b) Throw in additional stages, off-step points, super-future points and like. This leads into the large field general linear methods [8]. In this paper we use
derivatives of solutions up to third and super-future points for obtaining higher order A-stable multi-step methods.

2. A GENERAL FORM OF THIRD DERIVATIVE MULTI-STEP METHODS (TDMMs)

Let us consider the stiff initial value problem
\[ y'(x) = f(x, y(x)), \quad y(x_0) = y_0 \] (2.1)
on the bounded interval \( I = [x_0, x_N] \) where \( y : I \to \mathbb{R}^m \) and \( f : I \times \mathbb{R}^m \to \mathbb{R}^m \) is twice continuously differentiable function. The general TDMM can be written as:
\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} + h^2 \sum_{j=0}^{k} \gamma_j g_{n+j} + h^3 \sum_{j=0}^{k} \delta_j l_{n+j} \] (2.2)
where \( \alpha_j, \beta_j, \gamma_j, \delta_j \) are parameters to be determined and \( g(x, y) = y''(x), \ l(x, y) = y'''(x) \). If at least one of the parameters \( \beta_k, \gamma_k \) and \( \delta_k \) be nonzero then the method (2.2) is implicit. By using Taylor expansion we see that the method (2.2) is of order \( p \) if and only if
\[ \sum_{j=0}^{k} \alpha_j j^q = q \sum_{j=0}^{k} \beta_j j^{q-1} + q(q-1) \sum_{j=0}^{k} \gamma_j j^{q-2} + q(q-1)(q-2) \sum_{j=0}^{k} \delta_j j^{q-3} \] (2.3)
with \( 3 \leq q \leq p \).

3. THIRD DERIVATIVE BACKWARD DIFFERENTIATION FORMULAE (TDBDF)

We now introduce TDBDF that has the general form:
\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h \beta_k f_{n+k} + h^2 \gamma_k g_{n+k} + h^3 \delta_k l_{n+k} \] (3.1)
where \( \alpha_k = 1 \) and the other coefficients are chosen so that (3.1) be of order \( k + 2 \). The coefficients of \( k \)-step methods (3.1) for \( k = 1, 2, \cdots, 6 \) are given in Table 1.

<table>
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3.1. Stability analysis. If we apply (3.1) to the test problem \( y' = \lambda y \) for which \( y'' = \lambda^2 y \) and \( y''' = \lambda^3 y \), we get \( k \sum_{j=0}^{k} C_j(\bar{h})y_{n+j} = 0 \) where \( \bar{h} = \lambda h \), \( C_k(\bar{h}) = 1 - \bar{h}\beta_k - \bar{h}^2\gamma_k - \bar{h}^3\delta_k \) and \( C_j(\bar{h}) = \alpha_j \) for \( j = 0, 1, \cdots, k - 1 \). Therefore, the corresponding characteristic equation of the \( k \)th order difference equation of the method (3.1) is

\[
\pi(\xi, \bar{h}) = \sum_{j=0}^{k} C_j(\bar{h})\xi^j = 0. \tag{3.2}
\]

To see the zero-stability of this method, one can easily show that by substituting \( \bar{h} = 0 \) in (3.2) the resulted characteristic polynomial satisfies the root condition and so the method for \( k = 1, 2, \cdots, 14 \) is zero-stable.

To obtain the region of absolute stability we use the boundary locus method. By using coefficients of different powers of \( \bar{h} \) in (3.2), we obtain

\[
A_3\bar{h}^3 + A_2\bar{h}^2 + A_1\bar{h} + A_0 = 0 \tag{3.3}
\]

where \( A_0 = \xi^k + \sum_{j=0}^{k-1} \alpha_j \xi^j, \ A_1 = -\beta_k \xi^k, \ A_2 = -\gamma_k \xi^k \) and \( A_3 = -\delta_k \xi^k \). Inserting \( \xi = e^{i\theta}, \ (3.3) \) gives us three roots \( \tilde{h}_i(\theta), \ i = 1, 2, 3 \) which describe the stability domain. The method (3.1) is \( A \)–stable for \( k = 2, 3, 4 \), and it is \( A(\alpha) \)–stable for \( k = 5, 6, \cdots, 14 \). The corresponding (approximate) region of \( A(\alpha) \)–stability found using a numerical approach are given in Table 3 and Figures 1, 2. The method (3.1)

![Figure 1. The boundary of the stability region of method (3.1) for k = 2, 3, 4.](image_url)
4. Extended Third Derivative Backward Differentiation Formula (ETDBDF)

We now introduce an extended TDBDF that has the general form:

\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h \dot{\alpha}_k \dot{f}_{n+k} + h^2 \dot{\gamma}_k g_{n+k} + h^3 (\delta_k l_{n+k} - \dot{\delta}_{k+1} l_{n+k+1}) \] (4.1)

where \( g(x, y) = y''(x) \), \( l(x, y) = y'''(x) \), \( \dot{\alpha}_k = 1 \) and the other coefficients are chosen so that (4.1) be of order \( k + 3 \). The coefficients of \( k \)-step methods (4.1) for \( k = 1, 2, \ldots, 6 \) are given in Table 2. In this method we use the one super-future point technique.

Assume that the solution values \( y_n, y_{n+1}, \ldots, y_{n+k-1} \) are available. The method (4.1) is used to solve differential equation (2.1) by the following stages.

**Stage 1.** Compute \( \bar{y}_{n+k} \) as the solution of

\[ \sum_{j=0}^{k-1} \alpha_j \bar{y}_{n+j} + \alpha_k \bar{y}_{n+k} = h \dot{\alpha}_k \dot{f}_{n+k} + h^2 \dot{\gamma}_k \bar{g}_{n+k} + h^3 \delta_k \bar{l}_{n+k} \] (4.2)
Stage 2. Compute $\bar{y}_{n+k+1}$ as the solution of
\begin{equation}
\sum_{j=0}^{k-2} \alpha_j y_{n+j+1} + \alpha_{k-1} \bar{y}_{n+k} + \alpha_k \bar{y}_{n+k+1} = h^3 \beta_k \bar{f}_{n+k+1} + h^2 \gamma_k \bar{g}_{n+k+1} + h^3 \delta_k \bar{l}_{n+k+1},
\end{equation}
where $\bar{f}_{n+k} = f(x_{n+k}, \bar{y}_{n+k})$, $\bar{g}_{n+k} = g(x_{n+k}, \bar{y}_{n+k})$, $\bar{l}_{n+k} = l(x_{n+k}, \bar{y}_{n+k})$, $\alpha_k = 1$ and the other coefficients are chosen so that (4.2) has order $k + 2$. The coefficients of k-step methods of class (4.2) are given in Table 1, for $k = 1, 2, \cdots, 6$.

Stage 3. Compute $y_{n+k}$ by
\begin{equation}
\sum_{j=0}^{k} \alpha_j y_{n+j} = h^3 \beta_k \bar{f}_{n+k} + h^2 \gamma_k \bar{g}_{n+k} + h^3 (\delta_k l_{n+k} - \delta_{k+1} \bar{l}_{n+k+1}).
\end{equation}

Theorem 4.1. In order to method introduced in (4.1) we have
(i) Relation (4.2) is of order $k + 2$.
(ii) Relation (4.1) is of order $k + 3$.
(iii) If the implicit algebra equations defining $\bar{y}_{n+k}$, $\bar{y}_{n+k+1}$ are solved exactly, then the scheme (4.4) is of order $k + 3$.

Proof. Suppose the values $y_n, y_{n+1}, \cdots, y_{n+k-1}$ be exact. From (4.2) we have
\begin{equation}
y(x_{n+k}) - \bar{y}_{n+k} = C_1 h^{k+3} y^{(k+3)}(x_{n+k}) + O(h^{k+4}).
\end{equation}
From (4.5) for one super-future point and if we suppose that $y(x_{n+k}) = y_{n+k}$ we have
\begin{align*}
y(x_{n+k+1}) - \bar{y}_{n+k+1} &= C_1 h^{k+3} y^{(k+3)}(x_{n+k+1}) + O(h^{k+4}) \\
&= C_1 h^{k+3} y^{(k+3)}(x_{n+k}) + C_1 h^{k+4} y^{(k+4)}(x_{n+k}) + O(h^{k+4}).
\end{align*}
But since in (4.3) we apply \( \bar{y}_{n+k} \), we must add the error of \( (y(x_{n+k}) - \bar{y}_{n+k}) \) to the above expression. Hence

\[
y(x_{n+k+1}) - \bar{y}_{n+k+1} = C_1(1 - \alpha_{k-1})h^{k+3}y^{(k+3)}(x_{n+k}) + O(h^{k+4}).
\]  

(4.6)

If \( C_2h^{k+4}y^{(k+4)}(x_{n+k}) + O(h^{k+5}) \) be the defect of formula (4.5) then by replacing \( l(x_{n+k+1}, y(x_{n+k+1})) \) with \( l(x_{n+k+1}, \bar{y}_{n+k+1}) \) and adding the expression obtained in (4.6) to this error we get

\[
y(x_{n+k}) - y_{n+k} = C_2h^{k+4}y^{(k+4)}(x_{n+k}) - h^3\delta_{k+1}[l(x_{n+k+1}, y(x_{n+k+1})) - l(x_{n+k+1}, \bar{y}_{n+k+1})]. \]

Also from (4.6) we have

\[
C_1(1 - \alpha_{k-1})h^{k+3}y^{(k+3)}(x_{n+k}) + O(h^{k+4}).
\]

This yields

\[
y(x_{n+k}) - y_{n+k} = h^{k+4}[C_2y^{(k+4)}(x_{n+k}) - \frac{\partial l}{\partial y}(x_{n+k+1}, \eta)C_1(1 - \alpha_{k-1})h^{k+3}y^{(k+3)}(x_{n+k})] + O(h^{k+5})
\]

which shows that the order of scheme (4.4) is \( k + 3 \).

\[\square\]

**Remark 4.2.** The class of ETDMM methods are 3-stage methods therefore to reduce the implementation cost of ETDBDFs, we consider the stage 3 as follows:

**Stage 3**. Compute \( y_{n+k} \) by

\[
y_{n+k} - h\beta_k\bar{f}_{n+k} - h^2\gamma_kg_{n+k} - h^3\delta_kl_{n+k} = -\sum_{j=0}^{k-1}\hat{\alpha}_jy_{n+j}
\]

(4.7)

\[+h(\hat{\beta}_k - \beta_k)\bar{f}_{n+k} + h^2(\hat{\gamma}_k - \gamma_k)\bar{g}_{n+k} + h^3(\hat{\delta}_k - \delta_k)\bar{l}_{n+k} + h^3\delta_{k+1}\bar{l}_{n+k+1}.
\]

Therefore, the Jacobian matrix in each of the 3 stages (1), (2) and (3*) is the same as \( I - h\beta_k\frac{\partial f}{\partial y} - h^2\gamma_k\frac{\partial g}{\partial y} - h^3\delta_k\frac{\partial l}{\partial y} \).

4.1. **Stability analysis.** We now examine the stability of our method. If we apply (4.2) and (4.4) to the test problem \( y' = \lambda y \) for which \( y'' = \lambda^2 y \) and \( y''' = \lambda^3 y \), we get

\[
\sum_{j=0}^{k} C_j(h)\bar{y}_{n+j} = 0
\]

(4.8)

where

\[
\bar{h} = \lambda h , \quad A = 1 - \bar{h}\beta_k - \bar{h}^2\gamma_k - \bar{h}^3\delta_k,
\]

\[
d_0 = \frac{\alpha_0\alpha_{k-1}}{A_k} , \quad d_j = \frac{\alpha_j\alpha_{k-1}}{A_k} - \frac{\alpha_{j-1}}{A_k} , \quad j = 1, 2, \ldots, k - 1,
\]

\[
C_k = 1 - \bar{h}\beta_k - \bar{h}^2\gamma_k - \bar{h}^3\delta_k , \quad C_j = \hat{\alpha}_j + \bar{h}^3\delta_{k+1}d_j , \quad j = 0, 1, \ldots, k - 1.
\]

Therefore the corresponding characteristic equation of the \( k \)th order difference equation of the method (4.1) is

\[
\pi(\xi, \bar{h}) = \sum_{j=0}^{k} C_j(\xi - \hat{\alpha}_j) = 0
\]

(4.9)
To see the zero-stability of this method, one can easily show that by substituting \( \bar{h} = 0 \) in (4.9) the resulted characteristic polynomial satisfies the root condition and so the method is zero-stable. For more details see [5, 8].

**Table 3.** \( A(\alpha) \)–stability of TDMM method

<table>
<thead>
<tr>
<th>( k )</th>
<th>( p )</th>
<th>( \alpha(\circ) )</th>
<th>( k )</th>
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**Table 4.** \( A(\alpha) \)–stability of ETDBDF

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**Table 5.** \( A(\alpha) \)–stability of Ezzeddine method

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To obtain the region of absolute stability we use the boundary locus method. By using coefficients of different powers of \( \bar{h} \) in (4.9), we obtain

\[
\sum_{j=0}^{9} A_j \bar{h}^j = 0
\]  

(4.10)
where $A_j, j = 0, 1, \cdots, 9$ are functions of $\xi$ and $k$. Inserting $\xi = e^{i\theta}$, Eq. (4.10) gives nine roots $\tilde{h}_i(\theta), i = 1, 2, \cdots, 9$ which describe the stability domain. The corresponding (approximate) region of $A(\alpha)$–stability found using a numerical approach are given in Table 4.

**Remark 4.3.** Comparison of Tables 3, 4 and 5 shows that the regions of $A(\alpha)$–stability for our methods are larger than the Ezzeddine's method. The method (4.1) has the largest $A(\alpha)$–stability region in the introduced multi-step methods until now. For more details see, [1, 2, 3, 4, 5, 6, 9, 10].

5. **Numerical result**

We can see the numerical results of our method in the following examples.

**Example 5.1.** Consider the following stiff initial value problem:

\[
\begin{align*}
y_1' &= -\alpha y_1 - \beta y_2 + (\alpha + \beta - 1)e^{-x} \\
y_2' &= \beta y_1 - \alpha y_2 + (\alpha - \beta - 1)e^{-x}
\end{align*}
\]

with initial value $y(0) = (1, 1)^T$. The eigenvalues of the Jacobine associated with the resulting system are $-\alpha + i\beta, -\alpha - i\beta$ and the required solution is $y_1(x) = y_2(x) = e^{-x}$. The error results for $\alpha = 1$ and $\beta = 15$ are shown in Table 6.

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<td>$1.9 \times 10^{-21}$</td>
<td>$4.2 \times 10^{-19}$</td>
<td>$1.52 \times 10^{-22}$</td>
</tr>
</tbody>
</table>

**Example 5.2.** Let us consider the system of differential equations as follows:

\[
\begin{align*}
y_1' &= -20y_1 - 0.25y_2 - 19.75y_3, \\
y_2' &= 20y_1 - 20.25y_2 + 0.25y_3, \\
y_3' &= 20y_1 - 19.75y_2 - 0.25y_3,
\end{align*}
\]

with $y(0) = (1, 0, -1)$ and theoretical solution

\[
\begin{align*}
y_1 &= \frac{1}{2}(e^{-0.5x} + e^{-20x}(\cos(20x) + \sin(20x))), \\
y_2 &= \frac{1}{2}(e^{-0.5x} - e^{-20x}(\cos(20x) - \sin(20x))), \\
y_3 &= \frac{1}{2}(e^{-0.5x} + e^{-20x}(\cos(20x) - \sin(20x))).
\end{align*}
\]
We solve this problem at $x = 10, 20, 30$ with $h = 0.01$ and $k = 4$ and compared the results with those of Ezzeddine’s method [6]. The results tabulate in Table 7.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$y_i$</th>
<th>$ETDBDF$</th>
<th>$TDBDF$</th>
<th>Ezzeddine's method</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$y_1$</td>
<td>$7.5 \times 10^{-22}$</td>
<td>$1.1 \times 10^{-21}$</td>
<td>$5.8 \times 10^{-20}$</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>$7.5 \times 10^{-22}$</td>
<td>$1.1 \times 10^{-21}$</td>
<td>$5.8 \times 10^{-20}$</td>
</tr>
<tr>
<td></td>
<td>$y_3$</td>
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<td>$1.1 \times 10^{-21}$</td>
<td>$5.8 \times 10^{-20}$</td>
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<td>20</td>
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<td>$1.0 \times 10^{-23}$</td>
<td>$1.3 \times 10^{-23}$</td>
<td>$8.0 \times 10^{-22}$</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>$1.0 \times 10^{-23}$</td>
<td>$1.3 \times 10^{-23}$</td>
<td>$8.0 \times 10^{-22}$</td>
</tr>
<tr>
<td></td>
<td>$y_3$</td>
<td>$1.0 \times 10^{-23}$</td>
<td>$1.3 \times 10^{-23}$</td>
<td>$8.0 \times 10^{-22}$</td>
</tr>
<tr>
<td>30</td>
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<td>$1.2 \times 10^{-25}$</td>
<td>$8.2 \times 10^{-24}$</td>
</tr>
<tr>
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<td>$1.2 \times 10^{-25}$</td>
<td>$8.2 \times 10^{-24}$</td>
</tr>
<tr>
<td></td>
<td>$y_3$</td>
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<td>$1.2 \times 10^{-25}$</td>
<td>$8.2 \times 10^{-24}$</td>
</tr>
</tbody>
</table>

6. Conclusion

In this paper two class of third derivative multi-step methods (TDMMs) with good stability properties have been introduced. We discussed stability analysis of these methods. Comparing $A(\alpha)$—stability region of our methods with the presented methods showed that our methods have the largest $A(\alpha)$—stability region.

References