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On the stability functions of second derivative implicit advanced-step point methods

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Abstract. In the construction of efficient numerical methods for the stiff initial value problems, some second derivative multistep methods have been introduced equipping with super future point technique. In this paper, we are going to introduce a formula for the stability functions of a class of such methods. This group of methods encompasses SDBDF methods and their extensions with advanced step-point feature. This general formula, instead of obtaining the distinct stability functions for each of methods, will facilitate stability analysis of the methods.

Keywords: Initial value problem, second derivative methods, stability function, advanced-step point methods, stiff systems.
AMS Subject Classification 2010: 65L05.

1 Introduction

Several attempts have been made to derive efficient numerical methods for solving stiff initial value problems (IVPs) in ordinary differential equations (ODEs)

$$\begin{aligned} y'(x) &= f(x, y(x)), \qquad x \in [t_0, X], \\ y(x_0) &= y_0, \end{aligned} \tag{1}$$

where $f : \mathbb{R}^m \to \mathbb{R}^m$ and m is the dimensionality of the system. Most of the constructed methods in the class of linear multistep methods (LMMs) are improvements on backward differentiation formulae (BDF) by using some techniques such as higher derivatives of the solutions, off-step points and super future points. Extended BDF methods (EBDF) which utilizes a future point was introduced by Cash [8] to improve the stability properties and pass Dahlquist second barrier [12] on the existing A-stable methods. EBDF methods were modified to MEBDF (modified EBDF) [10] and MF-MEBDF (matrix free MEBDF)

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methods [20] to optimize the necessary computations of EBDF. Also, to increase the stability region, by inserting a free parameter in BDF and EBDF algorithms, the blended methods A-BDF [15] and A-EBDF [18] were introduced.

Among the main directions in searching for higher order A-stable methods, the use of the second derivative of the solution has been one of the effective techniques for the construction of methods of higher order with extensive region of stability. Second derivative multistep methods (SDMMs) introduced by Enright [13] and second derivative BDF methods (SDBDF) [16] were the first second derivative LMMs, meanwhile they have been also base for other modifications of second derivative methods in this class. Using of the second derivative of the solution has been also successfully applied to Runge–Kutta methods to introduce TDRK methods [11, 22]. Second derivative general linear methods (SGLMs) as a unifying framework for the traditional methods incorporating second derivative of the solution were introduced by Butcher and Hojjati in [7] and were studied more by Abdi and Hojjati in [3–5] to study the properties of the methods and to formulate new methods with clear advantages over the traditional ones. For more details of SGLM one can see [1, 2, 6].

The SDMMs equipped with super future point technique have led to successful methods. A set of second derivative extended backward differentiation formulas (E2BD) was derived by Cash [9] in two classes which are very highly stable. Considering these methods from SGLMs point of view, made it possible to improve their stability properties by introducing new classes of methods, so-called ME2BD, PME2BD and FPME2BD, with the same order but more extensive region of absolute stability [21]. A class of SDMMs equipped with the super future point technique based on SDBDF methods, so called ESDMMs, and their modification, MESDMMs, were constructed in [19]. Furthermore, some perturbations of these methods which improve their stability properties while preserve their order, were studied in [14]. In an another attempt, to implement the methods in parallel computers, a scheme was investigated in [17] based on SDBDF possessing super future point technique, so-called PMESDMM, which let them be faster on the vast majority of the problem.

For each of the above-mentioned methods analyzing the stability properties goes through the increasingly complicated calculations. In this paper, we are going to derive a general formula that generates the stability functions of the implicit advanced step-point SDMMs (IASS) encompassing SDBDF, ESDMM, MESDMM and PMESDMM. Such general formulae can provide us with a glimpse of the theoretical and computational difficulties encountered during the investigation of multi-stage methods. Also, the study on this general formula for the stability functions of the mentioned class of methods can assist in maneuvering on the structure of the methods to introduce methods with improved stability properties. A similar general formula for a group of implicit advanced step-point methods incorporating only the first derivative of the solution has been given in [23].

After the present introduction, a briefly review on general form of SDMMs and conventional SDBDF methods is given in Section 2. In Section 3, the stability analysis of MESDMMs are discussed and the stability functions of each method in the class of IASS methods are individually obtained. Section 4 is devoted to introduce a general formula which generates the stability functions of SDBDF and IASS methods. Finally, the paper is closed by giving some concluding remarks in Section 5.

2 A review on the SDMMs

A k-step SDMM in general form for solving (1) can be written as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} + h^2 \sum_{j=0}^{k} \gamma_j g_{n+j}, \qquad n = 0, 1, \ldots, N-k, \tag{2}$$

where α_j, β_j and γ_j are parameters to be determined. The SDMM (2) is implicit if $\beta_k^2 + \gamma_k^2 \neq 0$. Here, y_{n+j} is an approximation to the solution of (1) at the point x_{n+j}, $f_{n+j} = f(x_{n+j}, y_{n+j})$, $g_{n+j} = g(x_{n+j}, y_{n+j})$ with $g(x,y) := y'' = f_x + f_y f$, h is the stepsize, and $Nh = X - x_0$. Using Taylor expansion it can be seen that the method (2) is of order p if and only if

$$\sum_{j=0}^{k} \alpha_j j^q = q \sum_{j=0}^{k} \beta_j j^{q-1} + q(q+1) \sum_{j=0}^{k} \gamma_j j^{q-2},$$

with $0 \leq q \leq p$. In the implementation of such methods, using of the second derivative of the solution does not impose additional computational cost; indeed, in the implementation of the implicit methods for stiff autonomous systems $y'(x) = f(y(x))$, to solve the obtained non-linear algebraic equations, we usually need to compute $\partial f / \partial y$, so the second derivative of the solution at the step points can be approximated by $g(y) = (\partial f / \partial y) f(y)$ without any additional computational cost [13].

2.1 The stability function of SDBDF

SDBDF methods, inspired from BDF, have been designed such that in which the structure of the stability function allows to get better absolute stability properties than general form of SDMMs. A k-step SDBDF takes the form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_k f(y_{n+k}) + h^2 \gamma_k g(y_{n+k}), \tag{3}$$

in which, $\alpha_k = 1$ and the other coefficients are chosen such that the method has order $p = k+1$. To analyze the linear stability behavior of the SDBDF (3), we apply the method to the standard test problem of Dahlquist [12]

$$y' = \lambda y, \qquad \lambda \in \mathbb{C}, \tag{4}$$

and get

$$\sum_{j=0}^{k} C_{SDBDF,j}(z) y_{n+j} = 0, \tag{5}$$

where $z = h\lambda$ and

$$\begin{aligned} C_{SDBDF,k}(z) &= 1 - z\beta_k - z^2 \gamma_k, \\ C_{SDBDF,j}(z) &= \alpha_j, \qquad\qquad j = 0, 1, \ldots, k-1. \end{aligned} \tag{6}$$

Therefore, the linear stability properties of the SDBDF methods are determined by the stability function

$$\Phi_{SDBDF}(w,z)=\sum_{j=0}^{k}C_{SDBDF,j}(z)w^{j}. \tag{7}$$

Now, the linear stability criterion of the SDBDF in terms of the roots of $\Phi(w,z)$ requires that all the roots $w_i = w_i(z)$, $i = 1,2,\dots,k$, lie inside the unit circle with only simple roots on the boundary. SDBDF methods are A-stable up to order $p = 4$ $(k = 3)$ and $A(\alpha)$-stable up to order $p = 11$ $(k = 10)$ [16]. So, by these methods the Dahlquist second barrier was passed. Similar to the directions of construction algorithms based on BDF, SDBDF methods because of their accuracy and stability properties, have been extended to some classes of reliable methods. A group of such methods, IASS methods, are reviewed from the point of view theie stability function in the next section. For the SDBDF methods, the stability function (7) is obtained easily, but as we will see in the next section, things become messier for IASS methods mentioned in Section 1.

3 The stability functions of IASS methods

In this section, we discuss the stability functions of IASS methods encompassing ESDMMs, MESDMMs and PMESDMMs. These group of the implicit schemes have been introduced in [17, 19]. The stability analysis of ESDMMs and PMESDMMs have been already studied and here we concisely recall the stability functions of these methods. For MESDMMs, we present a detailed account of the stability function which does not given in [19].

3.1 The stability function of ESDMMs

The ESDMM is an implicit scheme which uses two SDBDF predictors and one implicit SDMM corrector given by the formula

$$\sum_{j=0}^{k}\widehat{\alpha}_j y_{n+j}=h\widehat{\beta}_k f_{n+k}+h^2(\widehat{\gamma}_k g_{n+k}-\widehat{\gamma}_{k+1}g_{n+k+1}). \tag{8}$$

Here $\widehat{\alpha}_k = 1$ and the coefficients $\widehat{\alpha}_j$, $j = 0,1,\dots,k-1$, $\widehat{\beta}_k$, $\widehat{\gamma}_k$, $\widehat{\gamma}_{k+1}$ are chosen so that (8) has the order $p = k+2$. The coefficients of the k-step methods of class (8) are given in [19]. Assuming that the solution values of $y_n, y_{n+1},\dots,y_{n+k-1}$ are available, the ESDMM approach goes as follows:

- **Stage 1.** Use the SDBDF (3) as predictor to compute $\overline{y}_{n+k}$ as

$$\overline{y}_{n+k}+\sum_{j=0}^{k-1}\alpha_j y_{n+j}=h\beta_k\overline{f}_{n+k}+h^2\gamma_k\overline{g}_{n+k}, \tag{9}$$

  where $\overline{f}_{n+k} = f(x_{n+k},\overline{y}_{n+k})$ and $\overline{g}_{n+k} = g(x_{n+k},\overline{y}_{n+k})$.

- **Stage 2.** Use the SDBDF (3) as predictor to compute $\overline{y}_{n+k+1}$ as

$$\overline{y}_{n+k+1}+\alpha_{k-1}\overline{y}_{n+k}+\sum_{j=0}^{k-2}\alpha_j y_{n+j+1}=h\beta_k\overline{f}_{n+k+1}+h^2\gamma_k\overline{g}_{n+k+1}, \tag{10}$$

  where $\overline{f}_{n+k+1} = f(x_{n+k+1},\overline{y}_{n+k+1})$ and $\overline{g}_{n+k+1} = g(x_{n+k+1},\overline{y}_{n+k+1})$.

- **Stage 3.** Compute y_{n+k} as the solution of the corrector

$$y_{n+k} + \sum_{j=0}^{k-1} \widehat{\alpha}_j y_{n+j} = h\widehat{\beta}_k f_{n+k} + h^2(\widehat{\gamma}_k g_{n+k} - \widehat{\gamma}_{k+1}\overline{g}_{n+k+1}).$$

The overall k-step ESDMM is of order $p = k+2$. Applying the overall ESDMM to the Dahlquist test problem (4), we get

$$\sum_{j=0}^{k} C_{ESDMM,j}(z) y_{n+j} = 0, \tag{11}$$

with

$$\begin{aligned} C_{ESDMM,k}(z) &= 1 - z\widehat{\beta}_k - z^2\widehat{\gamma}_k, \\ C_{ESDMM,j}(z) &= \widehat{\alpha}_j + z^2\widehat{\gamma}_{k+1}\, d_j, \qquad j = 0,1,\ldots,k-1, \end{aligned} \tag{12}$$

in which $A = 1 - z\beta_k - z^2\gamma_k$ and

$$\begin{aligned} d_0 &= \frac{\alpha_0\alpha_{k-1}}{A^2}, \\ d_j &= \frac{\alpha_j\alpha_{k-1}}{A^2} - \frac{\alpha_{j-1}}{A}, \qquad j = 1,2,\ldots,k-1. \end{aligned} \tag{13}$$

Therefore, the stability function of ESDMMs scheme takes the form

$$\Phi_{ESDMM}(w,z) = \sum_{j=0}^{k} C_{ESDMM,j}(z) w^j. \tag{14}$$

ESDMMs are A-stable up to order $p = 6$ $(k = 4)$ and $A(\alpha)$-stable up to order $p = 14$ $(k = 12)$. Angles of $A(\alpha)$-stability of ESDMMs are reported in Table 2.

3.2 The stability function of MESDMMs

In each stage of ESDMM scheme, the algebraic equations are solved using a modified form of Newton. The Jacobian matrix for stages 1 and 2 is the same but it differs for Stage 3. In order to unify the Jacobin matrix in all three stages with the aim of reducing the computational cost, a modification of ESDMM, so-called MESDMM, was introduced in which the third stage is replaced by the following formula

- **Stage** $3^\star$. Compute y_{n+k} as the solution of the corrector

$$\begin{aligned} y_{n+k} + \sum_{j=0}^{k-1} \widehat{\alpha}_j y_{n+j} = {} & h(\widehat{\beta}_k - \beta_k)\overline{f}_{n+k} + h\beta_k f_{n+k} + h^2(\widehat{\gamma}_k - \gamma_k)\overline{g}_{n+k} \\ & - h^2\widehat{\gamma}_{k+1}\overline{g}_{n+k+1} + h^2\gamma_k g_{n+k}. \end{aligned} \tag{15}$$

This modification does not affect on the order of methods while there is an improvement on the stability regions for all values of k in MESDMMs.

The stability analysis MESDMMs has not been discussed in [19], so we study it here. Using of the test problem (4) and substituting it into the first predictor (9) gives

$$\overline{y}_{n+k} = -\frac{1}{A}\sum_{j=0}^{k-1} \alpha_j y_{n+j}, \tag{16}$$

and into the second predictor (10), also using (16), gives

$$\overline{y}_{n+k+1} = \sum_{j=0}^{k-1} d_j y_{n+j}, \tag{17}$$

where the coefficients d_j are given by (13). Now, by applying the corrector (15) to the test problem (4), using (16) and (17), we get the difference equation

$$\sum_{j=0}^{k} C_{MESDMM,j}(z) y_{n+j} = 0, \tag{18}$$

in which

$$\begin{aligned} C_{MESDMM,k}(z) &= 1 - z\beta_k - z^2\gamma_k, \\ C_{MESDMM,j}(z) &= \widehat{\alpha}_j + \frac{z(\widehat{\beta}_k - \beta_k) + z^2(\widehat{\gamma}_k - \gamma_k)}{A}\alpha_j + z^2\widehat{\gamma}_{k+1} d_j, \qquad j = 0,1,\ldots,k-1. \end{aligned} \tag{19}$$

Therefore, the stability function of MESDMMs scheme takes the form

$$\Phi_{MESDMM}(w,z) = \sum_{j=0}^{k} C_{MESDMM,j}(z) w^j. \tag{20}$$

Angles of $A(\alpha)$-stability of MESDMMs which are larger than those of ESDMMs are reported in Table 2.

3.3 The stability function of PMESDMMs

A class of methods possessing a parallel feature has been introduced in [17]. These three-stage methods which are based on MESDMMs, so-called PMESDMMs, may grant the possibility of their efficiently using on a parallel computer. Assuming that the solution values $y_n, y_{n+1}, \ldots, y_{n+k-1}$ are available, the PMESDMMs take the following form

- **Stage 1.** Use the SDBDF (3) as predictor to compute $\overline{y}_{n+k}$.
- **Stage 2.** Use the following predictor to compute $\overline{y}_{n+k+1}$

$$\overline{y}_{n+k+1} + \sum_{j=0}^{k-1} \overline{\alpha}_j y_{n+j} = h\overline{\beta}_{k+1} f(x_{n+k+1}, \overline{y}_{n+k+1}) + h^2\overline{\gamma}_{k+1} g(x_{n+k+1}, \overline{y}_{n+k+1}), \tag{21}$$

where the coefficients $\overline{\alpha}_j$, $j = 0,1,\ldots,k-1$, $\overline{\beta}_{k+1}$ and $\overline{\gamma}_{k+1}$, reported in [17], are chosen so that (21) has order $k+1$.

- **Stage 3.** Compute the corrected solution y_{n+k} using (15).

The parallel feature is because of independent of the second predictor of the first one. The overall k-step PMESDMMs is of order $p = k+2$. The numerical experiments reported in [17] indicate that the accuracy of the PMESDMMs is very satisfactory. Even a little improvement happens in the stability properties of PMESDMMs respect to MESDMMs.

Applying the overall PMESDMM to the test problem (4), we get

$$\sum_{j=0}^{k} C_{PMESDMM,j}(z) y_{n+j} = 0, \tag{22}$$

with

$$\begin{aligned} C_{PMESDMM,k}(z) &= 1 - z\beta_k - z^2\gamma_k, \\ C_{PMESDMM,j}(z) &= \widehat{\alpha}_j + \frac{z(\widehat{\beta}_k - \beta_k) + z^2(\widehat{\gamma}_k - \gamma_k)}{A}\alpha_j - \frac{z^2\widehat{\gamma}_{k+1}}{\overline{A}}\overline{\alpha}_j, \qquad j = 0,1,\ldots,k-1. \end{aligned} \tag{23}$$

in which $\overline{A} = 1 - z\overline{\beta}_{k+1} - z^2\overline{\gamma}_{k+1}$. Therefore, the stability function of PMESDMMs scheme takes the form

$$\Phi_{PMESDMM}(w,z) = \sum_{j=0}^{k} C_{PMESDMM,j}(z) w^j. \tag{24}$$

Angles of $A(\alpha)$-stability of PMESDMMs are reported in Table 2. PMESDMMs are A-stable up to order $p = 6$ $(k = 4)$ and $A(\alpha)$-stable up to order $p = 14$ $(k = 12)$.

4 A general formula for the stability functions of SDBDF and IASS methods

In the previous sections, the stability functions of SDBDF and IASS methods were given individually. As it is seen, this investigation needs complicated calculations when the algorithm is multi-stage because of using future point technique. In this section, we introduce a general formula which generates the stability functions of SDBDF and IASS methods without needing to go through the increasingly complicated calculations for each case.

Theorem 1. *Suppose that*

i) α_j, β_k *and* γ_k *are the coefficients of SDBDF* (3)*;*

ii) $\widehat{\alpha}_j$, $\widehat{\beta}_k$, $\widehat{\gamma}_k$ *and* $\widehat{\gamma}_{k+1}$ *are the coefficients of ESDBDF* (8)*;*

iii) $\overline{\alpha}_j$, $\overline{\beta}_{k+1}$ *and* $\overline{\gamma}_{k+1}$ *are the coefficients of SDBDF* (21).

Then, for any permitted order and step-point k, the stability functions of the distinct schemes ESDMMs, MESDMMs and PMESDMMs, collectively named IASS methods, together with the stability function of SDBDF method can be obtained from the general formula

$$\Phi(w,z) = \sum_{j=0}^{k} C_j(z) w^j, \tag{25}$$

where

$$C_k(z) = 1 - z(\beta_k + b_k) - z^2(\gamma_k + c_k),$$
$$C_j(z) = \Big(1 - \theta + \mu \frac{z(\widehat{\beta}_k - \beta_k) + z^2(\widehat{\gamma}_k - \gamma_k)}{A}\Big)\alpha_j + \theta\widehat{\alpha}_j + \theta z^2 \overline{\gamma}_{k+1}\Big(\nu d_j + \frac{(\nu-1)\overline{\alpha}_j}{\overline{A}}\Big), \tag{26}$$

in which the other coefficients for each method are given in Table 1. The largest values of step-point k for SDBDF and IASS methods take $k = 10$ and $k = 12$, respectively.

Table 1: The coefficients in (26).

	b_k	c_k	θ	μ	ν
SDBDF	0	0	0	0	free
ESDMMs	$\widehat{\beta}_k - \beta_k$	$\widehat{\gamma}_k - \gamma_k$	1	0	1
MESDMMs	0	0	1	1	1
PMESDMMs	0	0	1	1	0

Proof. For the proof, one can obtain the stability function for each of the mentioned methods separately by the standard linear stability analysis and then verify the general formula (25) with the coefficients (26). □

The general formula given in Theorem 1 provides the expected results for the stability functions which can be of substantial assistance in stability analysis of the methods. Also, by using this general formula and developing a MATLAB code, one can plot the stability regions and drive the angles of $A(\alpha)$-stability of the methods. In Table 2, we report the angles of $A(\alpha)$-stability of SDBDF and IASS methods for $k = 1, 2, \ldots, 12$. Such a general formula is also important as they can provide ideas for designing new algorithms with better stability properties.

5 Conclusion

The stability properties of the numerical methods for stiff IVPs play an important role in the success of the methods. In the linear stability analysis of the methods, these properties are determined by their stability functions. For multi-stage methods which utilize the second derivative of the solution and equipped with the super future point technique, deriving the stability function requires complicated calculations. The introduced general formula for the stability functions IASS methods, as well as SDBDF, facilitates the stability analysis of these methods. Moreover, this formula can assist to follow that how maneuvering on the structure of the method can be useful in improving its stability properties.

Table 2: The angles of $A(\alpha)$-stability of SDBDF and IASS methods for $k = 1, 2, \ldots, 12$.

	SDBDF		ESDMM		MESDMM		PMESDMM	
k	p	α	p	α	p	α	p	α
1	2	90°	3	90°	3	90°	3	90°
2	3	90°	4	90°	4	90°	4	90°
3	4	90°	5	90°	5	90°	5	90°
4	5	89.36°	6	90°	6	90°	6	90°
5	6	86.35°	7	89.81°	7	89.86°	7	89.91°
6	7	80.82°	8	88.35°	8	88.49°	8	88.66°
7	8	72.53°	9	85.28°	9	85.83°	9	85.74°
8	9	60.71°	10	80.47°	10	80.81°	10	81.02°
9	10	43.39°	11	73.58°	11	76.34°	11	76.21°
10	11	12.34	12	63.98°	12	69.19°	12	64.75°
11	12	——	13	50.36°	13	59.37°	13	51.50°
12	13	——	14	29.90°	14	44.24°	14	31.55°

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