



On overcoming Dahlquist's second barrier for A -stable linear multistep methods

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Abstract

Dahlquist's second barrier limits the order of A -stable linear multistep methods to at most two, posing significant challenges for achieving higher accuracy in the numerical solution of stiff ordinary differential equations. Leveraging various successful techniques, many efforts have been made to develop efficient methods that overcome this fundamental obstacle through different approaches. In this paper, we survey these techniques and analyze their impact on enhancing the stability and accuracy of the resulting methods. A comprehensive understanding of these advances can assist researchers in designing more effective algorithms for stiff problems.

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1 Introduction

Stiff ordinary differential equations (ODEs) in the form

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

arise frequently in scientific and engineering applications where the solution exhibits components with widely varying time scales. Numerical solution of such systems requires methods that remain stable even when large step sizes are used for the rapidly decaying components. Explicit methods generally fail in this regard due to severe stability restrictions, making implicit methods the preferred choice for stiff problems. Among implicit methods, A -stable methods play a crucial role. A numerical method is said to be A -stable if its region of absolute stability contains the entire left half of the complex plane. This means that when applied to the standard test problem of Dahlquist [9]

$$y' = \lambda y, \quad \lambda \in \mathbb{C},$$

with $\operatorname{Re}(\lambda) < 0$, the numerical solution decays to zero for any stepsize $h > 0$, mirroring the behavior of the exact solution. This property ensures numerical stability for stiff problems without requiring small step sizes. To relax the stringent requirement of A -stability, the concept of $A(\alpha)$ -stability is introduced. A method is $A(\alpha)$ -stable if its region of absolute stability contains a sector of the left half-plane bounded by two rays forming an angle 2α with the negative real axis. While not fully A -stable, such methods maintain strong stability properties for many stiff problems and can achieve higher order accuracy.

Implicit Runge–Kutta (IRK) methods can be constructed without theoretical limitations on order while preserving A -stability. For example, IRKs, such as those based on Gauss, Radau, and Lobatto quadratures, can attain arbitrarily high order while preserving A -stability [14, 20, 7]. However, these methods require solving nonlinear systems of equations involving multiple implicit stages at each time step which leads to significantly higher computational cost.

Linear multistep methods (LMMs) as a class of multistage and one-stage methods, by incorporating past solution values and their derivatives, construct higher-order polynomial approximations that increase the order of accuracy without requiring additional function evaluations at intermediate stages within each step. A classical k -step LMM for solving (1) is given by

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j},$$

where α_j and β_j are parameters to be determined, $y_{n+j} \approx y(x_{n+j})$, h is the stepsize, and $f_{n+j} = f(x_{n+j}, y_{n+j})$. LMMs despite generally having lower computational cost than Runge–Kutta methods, suffer severe degradation of stability as their order increases. In particular, the requirement of A -stability puts a severe limitation on LMMs, which limits their applicability to stiff problems when high order accuracy is required. This pessimistic restriction is known as Dahlquist's second barrier.

Theorem 1 (Dahlquist's second barrier [9]). The maximal order of an A -stable LMM is two, and the trapezoidal rule is the unique method achieving this order with the minimal error constant.

Circumventing Dahlquist's second barrier poses challenges for designing efficient A - or $A(\alpha)$ -stable methods of high orders for stiff ODEs within the multistep framework. Developing such methods has been carried out by equipping traditional LMMs with various advanced techniques. A comprehensive understanding of the strategies involved in developing techniques to circumvent Dahlquist's second barrier is essential, as it enables researchers to design more effective and stable numerical algorithms tailored for stiff differential equations. Drawing on the authors' experience with methods over-

coming Dahlquist's second barrier, this paper surveys the successful research directions. This survey fills an existing gap in the literature by providing a unified overview of methods that overcome Dahlquist's second barrier. It highlights and compares various advanced techniques and their combinations that have been proposed to enhance the stability and accuracy of LMMs for stiff ODEs. By doing so, it offers researchers a comprehensive understanding of the strengths and limitations of each approach and fosters the generation of novel ideas for further advancements.

The paper is organized along the following lines. Section 2 introduces the advanced step-point strategy, reviewing several efficient methods based on backward differentiation formulas (BDF) that utilize this technique. In section 3, adaptive methods are discussed with a presentation of methods that incorporate adaptivity to enhance stability and accuracy. Section 4 focuses on second derivative methods as a successful strategy for improving both accuracy and stability. It demonstrates how LMMs have been enhanced using this approach and surveys several proposed methods that surpass Dahlquist's second barrier. Finally, section 5 concludes the paper with a summary of the main findings and remarks on future research directions.

2 Advanced step-point strategy

BDF methods constitute a widely used family of implicit LMMs for the numerical solution of ODEs, particularly effective for stiff problems. Initially developed by Curtiss and Hirschfelder [8] and later formalized by Gear [13], the k -step BDF method is given by

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k f_{n+k}. \quad (2)$$

Here, $\alpha_k = 1$ and the other coefficients are chosen so that the method has order $p = k$. A k -step BDF is A -stable for $k = p = 2$ and $A(\alpha)$ -stable for $k = p = 3, 4, 5, 6$; orders beyond six lose zero-stability and are generally not used in practice. Due to their favorable balance of stability and accuracy, BDF methods serve as the foundation for many robust stiff ODE solvers

such as LSODE and VODE [24, 19]. However, as a subclass of LMMs, they inherit the drawback that they cannot be A -stable for orders greater than two. Using the advanced step-point technique is one of the efficient strategies to overcome this drawback. In this way, some implicit advanced step-point (IAS) methods based on BDF methods have been introduced.

2.1 EBDF methods

Cash [4] enhanced BDF methods by incorporating the advanced step-point strategy, leading to the development of extended BDF (EBDF). The k -step EBDF method takes the form [4]

$$y_{n+k} + \sum_{j=0}^{k-1} \bar{\alpha}_j y_{n+j} = h \left(\bar{\beta}_k f_{n+k} + \bar{\beta}_{k+1} f_{n+k+1} \right), \quad (3)$$

where the coefficients are chosen to achieve order $p = k + 1$. Knowing the solutions y_{n+j} at the past nodes x_{n+j} , for $j = 0, 1, \dots, k - 1$, the EBDF algorithm proceeds as follows:

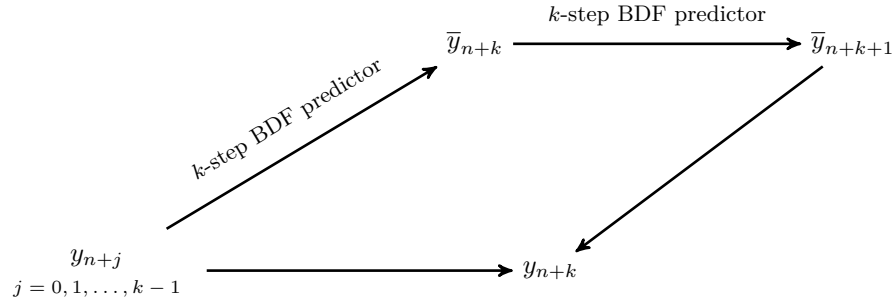
- The k -step BDF method predicts \bar{y}_{n+k} using y_{n+j} , $j = 0, 1, \dots, k - 1$.
- The k -step BDF method predicts \bar{y}_{n+k+1} using y_{n+j} , $j = 1, 2, \dots, k - 1$ and the predicted \bar{y}_{n+k} .
- Finally, the solution y_{n+k} is corrected using y_{n+j} , $j = 0, 1, \dots, k - 1$, and the predicted \bar{y}_{n+k+1} from (3) written in the form

$$y_{n+k} - h \bar{\beta}_k f_{n+k} = - \sum_{j=0}^{k-1} \bar{\alpha}_j y_{n+j} + h \bar{\beta}_{k+1} \bar{f}_{n+k+1},$$

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

The diagram of overall procedure of the EBDF methods has been plotted in Figure 1.

The EBDF methods are A -stable up to order *four* and $A(\alpha)$ -stable up to order *nine*, significantly improving the stability properties while achieving a higher order of convergence compared to classical BDF methods.

Figure 1: Diagram illustrating the k -step EBDf methods.

2.2 MEBDF methods

To avoid the need for computing and factorizing the two iteration matrices arising in the application of a modified Newton iteration at each stage—which leads to higher computational costs—EBDF approach was modified by Cash [6]. This modified method, known as the modified EBDf (MEBDF), replaces the corrector formula (3) with

$$y_{n+k} + \sum_{j=0}^{k-1} \bar{\alpha}_j y_{n+j} = h v_k \bar{f}_{n+k} + h(\bar{\beta}_k - v_k) f_{n+k} + h \bar{\beta}_{k+1} \bar{f}_{n+k+1}.$$

Here, the order of MEBDF is independent of the choice of v_k . Selecting $v_k = \bar{\beta}_k - \beta_k$, ensures that the coefficient matrix used in the modified Newton iteration scheme is the same for both the predictor and the corrector. This choice not only improves computational efficiency by requiring only one **LU** decomposition per step but also enlarges the $A(\alpha)$ -stability region compared to the original EBDf methods. The coefficients of the methods can be found in [4].

IAS methods have also been parallelized (so-called PIAS) aiming for significant efficiency gains and speed-ups, as shown by Psihoyios [22].

2.3 TIAS methods

The two implicit advanced step-point (TIAS) method, introduced by Psihoyios [22], extends the BDF family by incorporating two future points to improve accuracy and stability. The algorithm uses three predictor steps based on BDF and a corrector defined by

$$y_{n+k} + \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} = h \left(\hat{\beta}_k f_{n+k} + \hat{\beta}_{k+1} f_{n+k+1} + \hat{\beta}_{k+2} f_{n+k+2} \right). \quad (4)$$

Knowing the solutions y_{n+j} at the past nodes x_{n+j} , for $j = 0, 1, \dots, k-1$, the TIAS algorithm proceeds as follows:

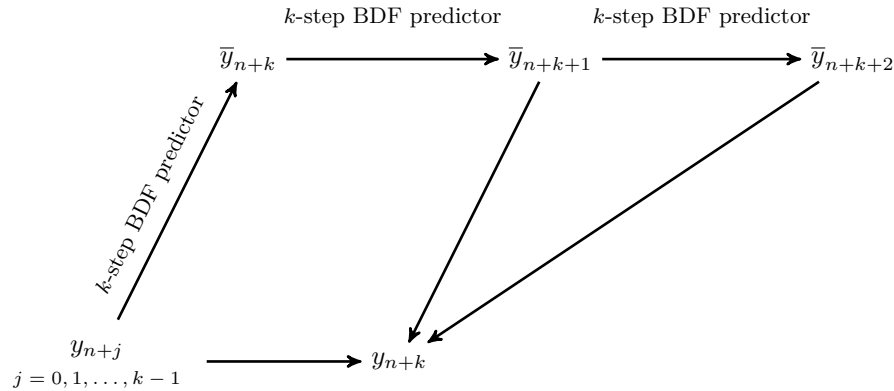
- The k -step BDF method predicts \bar{y}_{n+k} using y_{n+j} , $j = 0, 1, \dots, k-1$.
- The k -step BDF method predicts \bar{y}_{n+k+1} using y_{n+j} , $j = 1, 2, \dots, k-1$ and the computed \bar{y}_{n+k} .
- The k -step BDF method predicts \bar{y}_{n+k+2} using y_{n+j} , $j = 2, 3, \dots, k-1$ and the computed \bar{y}_{n+k} and \bar{y}_{n+k+1} .
- Finally, the TIAS corrector (4) computes the corrected solution y_{n+k} using y_{n+j} , $j = 0, 1, \dots, k-1$, and the predicted solutions \bar{y}_{n+k+1} and \bar{y}_{n+k+2} as

$$y_{n+k} - h\hat{\beta}_k f_{n+k} = - \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} + h\hat{\beta}_{k+1} \bar{f}_{n+k+1} + h\hat{\beta}_{k+2} \bar{f}_{n+k+2}.$$

The diagram of overall procedure of the TIAS methods has been plotted in Figure 2.

Using this approach, A -stable methods have been developed up to order *six*. However, this stability improvement was not achieved with the same level of optimization as in the MEBDF methods.

Considering the stability results of the classical BDF method (without advanced step-point) as well as those of methods with one and two advanced step-points aligns with the conjecture that the maximal order p of A -stable

Figure 2: Diagram illustrating the k -step TIAS methods.

methods increases with the number of advanced step-points, potentially following the relation:

$$p \leq 2q + 2,$$

where q is the number of advanced step-points. Based on the complexity involved in constructing A -stable methods of order six with $q = 2$, this conjecture has not yet been fully investigated [22].

A general formula was introduced in [23] that generates the stability functions of the methods BDF, EBDF, MEBDF, IAS, TIAS, and PIAS. This formula can substantially facilitate stability analysis and further computational manipulation of these and analogous schemes.

The features of the advanced step-point strategy have led to its application in the construction of other methods aimed at improving accuracy and stability properties. For example, Fazeli, Hojjati, and Shahmorad [11] introduced a class of multistep collocation methods for solving nonlinear Volterra integral equations, in which collocation points in the future interval, as well as in the current interval, are used. This technique results in high-order methods with an extensive absolute stability region.

3 Adaptive methods

Adaptive methods (also known as blended methods in some contexts) represent another effective technique for overcoming Dahlquist's second barrier. In this strategy, by incorporating adjustable parameters into the algorithms and tuning these to optimal values, the stability properties of the numerical methods can be significantly enhanced, enabling the construction of higher-order methods with improved absolute stability regions. This flexibility, when applied to LMMs, enables circumventing Dahlquist's second barrier.

3.1 AMF-BDF method

This strategy was first introduced by Skeel and Kong [25] by blending the k -step Adams–Moulton formula (AMF_k) and the k -step BDF (BDF_k) as

$$\text{AMF}_k - t h J \text{BDF}_k = 0,$$

in which $J = \frac{\partial f}{\partial y}$ is the Jacobian matrix of f with respect to y . This method is of order $p = k + 1$ for all values of t . The optimum values of t are given in [25]; see also [14], for which the method is A -stable up to order *four* and $A(\alpha)$ -stable up to order *twelve*, with larger values of α compared to the BDF method.

3.2 A-BDF method

The adaptive BDF (A-BDF), introduced by Fredebeul [12], generalizes the classical BDF methods by incorporating a parameter that can be optimized to improve stability properties. The k -step A-BDF method is a blended method of implicit and explicit BDF that can be expressed as

$$\text{A} - \text{BDF}_k(t) := \text{BDF}_k^{(i)} - t \text{BDF}_k^{(e)} = 0,$$

in which $\text{BDF}_k^{(i)}$ is the classical implicit k -step BDF (2), and $\text{BDF}_k^{(e)}$ is an explicit k -step BDF-type method defined by

$$\sum_{j=0}^k \alpha_j^* y_{n+j} = h\beta_{k-1}^* f_{n+k-1},$$

where $\alpha_k^* = 1$ and the other coefficients are chosen so that $\text{BDF}_k^{(e)}$ has order k . Therefore, a k -step A-BDF takes the form

$$\sum_{j=0}^k (\alpha_j - t\alpha_j^*) y_{n+j} = h\beta_k f_{n+k} - t\beta_{k-1}^* f_{n+k-1}.$$

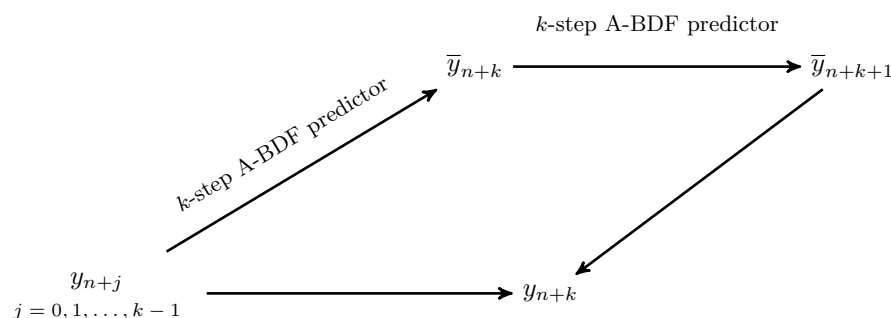
By finding the optimum values of the parameter t for each step number k , the maximum values of the angle α in $A(\alpha)$ -stability of A-BDF methods are achieved. The results reported in [12] show that the k -step A-BDF method is A -stable up to order *two* and $A(\alpha)$ -stable up to order *seven*, with larger values of α compared to the underlying classical k -step BDF.

3.3 A-EBDF method

The adaptive EBDF (A-EBDF), introduced by Hojjati, Rahimi Ardabili, and Hosseini [16], extends the A-BDF method to improve the stability properties of BDF, EBDF, and A-BDF. It combines two strategies—advanced step-point and adaptive methods—applied to the BDF algorithm. Knowing the solutions y_{n+j} at the past nodes x_{n+j} , $j = 0, 1, \dots, k-1$, the A-EBDF algorithm proceeds as follows:

- The k -step A-BDF method predicts \bar{y}_{n+k} using y_{n+j} , $j = 0, 1, \dots, k-1$.
- The k -step A-BDF method predicts \bar{y}_{n+k+1} using y_{n+j} , $j = 1, 2, \dots, k-1$ and the predicted \bar{y}_{n+k} .
- Finally, the k -step EBDF method (3) computes the solution y_{n+k} using y_{n+j} , $j = 0, 1, \dots, k-1$, and the predicted \bar{y}_{n+k+1} .

The diagram of overall procedure of the A-EBDF methods has been plotted in Figure 3.

Figure 3: Diagram illustrating the k -step A-EBDF methods.

It is proven that this scheme achieves order $k + 1$ for all values of the parameters $t \in \mathbb{R} \setminus \{1\}$. The optimum values of t resulting in the maximum angle α of $A(\alpha)$ -stability in A-EBDF are given in [16]. Stability analysis shows that the A-EBDF method is A -stable up to order *four* and $A(\alpha)$ -stable up to order *nine* with a larger angle α compared to the BDF, EBDF, and A-BDF methods. This improvement in stability properties results from the combination of the two aforementioned strategies applied to the BDF algorithm.

4 Second derivative methods

Incorporating the second derivative of the solution into numerical algorithms is an effective strategy to enhance both the accuracy and stability of the methods. Notably, in implicit methods, the use of the second derivative often incurs no additional computational cost. Specifically, for an autonomous problem of the form $y' = f(y)$, the second derivative can be expressed as $y'' = g = \frac{\partial f}{\partial y} f$, where $\frac{\partial f}{\partial y}$ is the Jacobian matrix of f . Also, for the Jacobian of g , a piecewise constant approximation of $(\frac{\partial f}{\partial y})^2$ is typically used.

The LMMs have been extended using this technique in many particular cases. A k -step second derivative linear multistep methods (SDMM) for the solution of the initial value problem (1) takes the general form

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} + h^2 \sum_{j=0}^k \gamma_j g_{n+j},$$

where $g := y'' = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f$ and $g_{n+j} = g(x_{n+j}, y_{n+j})$. In this section, we survey some efficient SDMMs and those combined with other techniques mentioned in previous sections.

4.1 SDBDF methods

Second derivative BDF (SDBDF) methods extend the classical BDF methods by incorporating the second derivative of the solution to improve accuracy and stability, particularly for stiff problems [14]. A k -step SDBDF method takes the form

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k f_{n+k} + h^2 \gamma_k g_{n+k}, \quad (5)$$

where $\alpha_k = 1$ and the other coefficients are chosen so that the method has order $p = k + 1$.

The inclusion of the second derivative term $h^2 \gamma_k g_{n+k}$ enhances the stability region of the method beyond that of classical BDF schemes. Notably, SDBDF methods are A -stable up to order *four* and $A(\alpha)$ -stable up to order *eleven* thereby surpassing Dahlquist's second barrier. Beyond serving as efficient solvers in their own right, SDBDF schemes play a foundational role—analogous to classical BDF methods—in the development of advanced numerical methods discussed later in this section.

4.2 Enright methods

These methods were introduced by Enright [10] by enhancing the Adams methods through incorporating the second derivative of the solution into the algorithm. The general form of a k -step Enright method is

$$y_{n+k} - y_{n+k-1} = h \sum_{j=0}^k \beta_j f_{n+j} + h^2 \gamma_k g_{n+k}, \quad (6)$$

where the coefficients are chosen so that the method has order $p = k + 2$.

Inheriting from Adams' methods, the zero-stability of these methods is guaranteed for all values of the step number k . The methods are A -stable up to order *four* ($k = 2$) and $A(\alpha)$ -stable up to order *nine* ($k = 7$), while for $k = 8$ the stability region becomes disconnected. It is worth noting that the underlying Adams–Moulton methods are A -stable only up to order two for $k = 0, 1$, and for other $k \geq 2$ the stability region is bounded.

4.3 E2BD methods

The second derivative extended backward differentiation formulas (E2BD) were introduced by Cash [5] as an enhancement of Adams-type methods by incorporating two key techniques: The use of an advanced step-point and the inclusion of the second derivative of the solution. These methods are typically implemented in a predictor-corrector mode and are classified into two main classes:

E2BD methods – Class 1

Predictor: The Enright method (6).

$$\text{Corrector: } y_{n+k} - y_{n+k-1} = h \sum_{j=0}^{k+1} \bar{\beta}_j f_{n+j} + h^2 (\bar{\gamma}_k g_{n+k} + \bar{\gamma}_{k+1} g_{n+k+1}). \quad (7)$$

In this class, the corrector extends the Enright method (6) by incorporating the first and second derivatives of the solution at the future point x_{n+k+1} . The coefficients in (7) are chosen to achieve order $p = k + 4$. A k -step E2BD method of Class 1, considering the predictor's order, attains overall

order $p = k + 3$. These methods exhibit superior stability properties, being A -stable up to order *eight*.

E2BD methods – Class 2

Predictor: The Enright method (6).

$$\text{Corrector: } y_{n+k} - y_{n+k-1} = h \sum_{j=0}^{k+1} \bar{\beta}_j f_{n+j} + h^2 \bar{\gamma}_k g_{n+k}. \quad (8)$$

In this class, only the second derivative of the solution at the future point x_{n+k+1} is incorporated in the corrector. The coefficients in (8) are chosen so that the method has order $p = k + 3$. Considering the predictor's order, a k -step E2BD method of Class 2 also has order $p = k + 3$. While these methods are computationally more efficient than those of Class 1, they exhibit slightly weaker stability properties, being A -stable up to order *six*.

Class 1 methods for $k \geq 6$ and Class 2 methods for $k \geq 4$, are $A(\alpha)$ -stable with large stability angles α . For example, the 6-step E2BD method of Class 1 has $\alpha > 89^\circ$. This makes these methods well-suited for integrating stiff differential systems whose Jacobians have eigenvalues with large imaginary components close to the imaginary axis.

4.4 ESDMMs

The extended SDMMs (ESDMMs) were introduced by Hojjati, Rahimi Ardabili, and Hossein [17] as an enhancement of the SDBDF methods by incorporating the second derivative of the solution at the future point into the algorithm. These methods can be also considered as an extension of BDF schemes employing two key strategies: The use of an advanced step-point and the inclusion of the second derivative of the solution. A k -step ESDMM has the general form

$$\sum_{j=0}^k \hat{\alpha}_j y_{n+j} = h\hat{\beta}_k f_{n+k} + h^2(\hat{\gamma}_k g_{n+k} - \hat{\gamma}_{k+1} g_{n+k+1}), \quad (9)$$

where $\hat{\alpha}_k = 1$ and the remaining coefficients are chosen to ensure the method attains order $p = k + 2$. Given the known solutions y_{n+j} at previous nodes x_{n+j} for $j = 0, 1, \dots, k - 1$, the ESDMM algorithm proceeds as follows:

- The k -step SDBDF (5) predicts \bar{y}_{n+k} using y_{n+j} , $j = 0, 1, \dots, k - 1$.
- The k -step SDBDF (5) predicts \bar{y}_{n+k+1} using y_{n+j} , $j = 1, 2, \dots, k - 1$ and the predicted \bar{y}_{n+k} .
- Finally, the k -step ESDMM (9) computes the solution y_{n+k} using y_{n+j} , $j = 0, 1, \dots, k - 1$, and the predicted \bar{y}_{n+k+1} as

$$y_{n+k} - h\hat{\beta}_k f_{n+k} - h^2\hat{\gamma}_k g_{n+k} = - \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} - h^2\hat{\gamma}_{k+1} \bar{y}_{n+k+1}.$$

The diagram of overall procedure of the ESDMMs has been plotted in Figure 4.

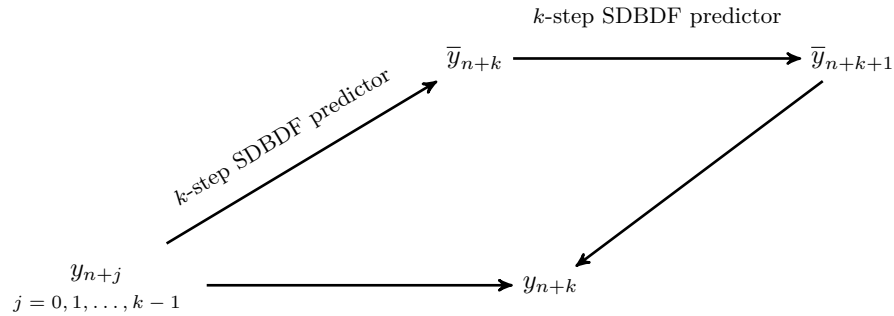


Figure 4: Diagram illustrating the k -step ESDMM methods.

ESDMMs exhibit A -stability up to order *six* and $A(\alpha)$ -stability up to order *fourteen*, with larger stability angles α compared to those of BDF and SDBDF methods.

In analogy with the motivation behind MEBDF methods, ESDMMs have been further refined into modified ESDMMs (MESDMMs) by replacing the corrector (9) with the following form [17]:

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

This modification not only reduces the computational cost associated with ESDMMs but also increases the stability angle α in the $A(\alpha)$ -stability property. MESDMMs have also been parallelized—referred to as PMESDMMs—to enable their efficient implementation on parallel computers [15].

A general formula introduced in [18] generates the stability functions for the SDBDF, ESDMMs, MESDMMs, and PMESDMMs. This formula helps to understand how modifying the structure of a method can effectively enhance its stability properties.

5 Conclusion

LMMs, as an efficient and flexible class of numerical methods for solving ODEs, face a significant challenge known as Dahlquist's second barrier, which limits their ability to solve stiff systems with high accuracy. This paper has investigated three effective strategies that overcome this barrier: Advanced step-point methods, adaptive methods and second derivative methods. These strategies can be applied individually or in combination to enhance LMMs. By analyzing their formulation and impact on stability, this study provides valuable insights for future research aimed at designing new and more robust algorithms. It is worth noting that other techniques, such as hybrid methods employing off-step points, also exist; however, the strategies discussed here represent general frameworks that generate entire classes of methods. Moreover, the first derivative methods, including LMMs, and second derivative methods, including SDMMs (and their modifications), are formulated within the general linear methods (GLMs) [3, 21] and second derivative GLMs (SGLMs) [1, 2] frameworks, respectively. Therefore, the strategies presented in this paper can be naturally extended to these more general frameworks.

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