

IMPLICIT-EXPLICIT SECOND DERIVATIVE LMM FOR STIFF ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT. The interest in implicit-explicit (*IMEX*) integration methods has emerged as an alternative for dealing in a computationally cost-effective way with stiff ordinary differential equations arising from practical modeling problems. In this paper, we introduce implicit-explicit second derivative linear multi-step methods (*IMEX* SDLMM) with error control. The proposed *IMEX* SDLMM is based on second derivative backward differentiation formulas (SDBDF) and recursive SDBDF. The *IMEX* second derivative schemes are constructed with order p ranging from $p = 1$ to 8. The methods are numerically validated on well-known stiff equations.

1. INTRODUCTION: IMEX METHODS AND THE PROTHERO-ROBINSON STIFF EQUATION

In many initial value problems of ordinary differential equations (ODEs)

$$y' = F(x, y(x)), \quad (1.1)$$

which arises from practical modelling, splitting the differential equations is necessitated naturally into two or more parts. One part of which is non-stiff or mildly stiff, and suitable for explicit time integration, and the other part is stiff and suited for implicit time integration. In this regard, the concern is the solution of the following ordinary differential equations (ODEs)

$$y' = f(x, y(x)) + g(x, y(x)), \quad y(0) = y_0, \quad (1.2)$$

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where $f(x, y(x))$ is a non-stiff term suitable for explicit time integration, for example advection term and $g(x, y(x))$ is a stiff term arising for an example from a diffusion term requiring an implicit time integration. The purpose is to avoid excessively small time integration steps. Models of (1.2) can be found for example in diffusion or chemical kinetics reaction, in discretization of advection–reaction equations [1, 2, 3]. The composition of implicit and explicit numerical methods employed to solve the system (1.2) is referred to as an implicit-explicit (IMEX) method, and it ensures the numerical stability of the solution of (1.2), while also reducing the difficulty of resolving the implicitness along with the computational effort of realizing this solution. These methods were introduced to solve partial differential equations (PDEs) in [4, 5, 6]. Derivation of the multi-step IMEX schemes and their stability properties is in [7, 8, 9, 10, 11, 12] and further analyzed in [13, 14]. Other methods of IMEX schemes such as the Runge-Kutta IMEX schemes are reported in [15, 16, 17, 18, 19, 20, 21, 22, 23, 24]. Implicit-explicit general linear methods have been proposed in [25, 26, 27, 28], while Super convergent IMEX peer methods can be found in [29, 30, 31]. Other numerical methods for solving Stiff ODEs include [32, 33, 34, 35, 36, 37].

However, it is not always simple to obtain stable IMEX scheme by coupling two multi-step methods. From an accuracy point of view, the minimum between the order of convergence of the coupled implicit and explicit methods give the effective order of accuracy of the overall IMEX method. An interesting class of problems suitable for IMEX schemes from equation (1.1) is the Prothero-Robinson equation [38] given by

$$y' = J(y(x) - u(x)) + u'(x), \tag{1.3}$$

where $u(x)$ is assumed to be slowly varying in the interval of integration and J denotes the variational matrix

$$J(x) = F_y(x, u(x)); \quad F_y = \frac{\partial F}{\partial y},$$

of the ODEs in (1.3). It does readily appear that $Jy(x)$ is the stiff part, while $-Ju(x) + u'(x)$ is the non-stiff part. Stiffness (see, [16], [39]), occur in equation (1.3), if the eigenvalues $\lambda(x)$ of the Jacobian matrix $J(x)$ are such that

$$\max_{\lambda} \left\{ Re(-\lambda(x)) \right\} \gg \max_{\lambda} \left\{ Re(\lambda(x)) \right\}, \tag{1.4}$$

for some value of x in the range of the solution $y(x)$. See other equivalent definitions of stiffness in [40, 41, 42]. The analysis of the stability and accuracy of one-step methods on the Prothero-Robinson stiff problem is in [38]. The (1.4) translate to the computational process in ([43],p. 50) of concluding stiffness of the ODE (1.3) through the stiffness ratio. However, stiffness has been identified as a transient behaviour of the ODE (1.3) by [44] and have therefore proposed that stiffness be characterize more appropriately by the pseudo-spectra

$$SP_{\epsilon}(J) = \left\{ \lambda : \|(J - \lambda I)^{-1}\| \geq \epsilon^{-1} \right\}$$

of J rather than by the spectra of J in (1.3), where ϵ is a positive real number. This set is a superset of the eigenvalues or spectra of J . In fact, the ODE (1.3) is stiff, for a fixed $x = x_0$ if the pseudo-spectral $SP_\epsilon(J)$ of J extend far into the left-half-plane (see, [44]). Even moreso, will the method have difficulties computing the solution of this ODE, if the pseudo-spectral region encroaches far into the stability region of the ODEs method in this half of the plane. In the case of (1.1) the Jacobian J is obtained from its linearisation, see [44]. This readily explains why explicit methods which are of bounded stability region on left half-plane are certainly not suitable for stiff problems of (1.1) and (1.2).

The paper is organized as follows. In section 2, a brief theory of second derivative linear multistep methods (SDLMM) is discussed and some recursively derived SDLMM based on SDBDF are given. The IMEX scheme is derived from SDBDF and its stability analysis is discussed in section 3. The error control and stepsize changing strategy is considered in section 4. The results of numerical experiments with the *IMEX* SDLMM are presented in section 5.

2. A THEORY OF SECOND DERIVATIVE LINEAR MULTISTEP METHODS

In an attempt to overcome the [45] order barrier for linear multistep method (LMM), [46] has considered the SDLMM though their order p is limited to $p = 4$ by the Daniel-Moore conjecture in ([42], p.286) for the A -stable ones, but are very ammenable to high order $A(\alpha)$ -stability properties. These methods are useful in dealing with stiff ODE (1.1) (see also, [46]). In this section we develop a theory and present further results on SDLMM. The SDLMM $[\rho(r), \sigma(r), \lambda(r)|k, p]$ of step number k and order p is

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j F_{n+j} + h^2 \sum_{j=0}^k \lambda_j F'_{n+j}, \quad (2.1)$$

employing the second derivative $y'' = F'(x, y(x)) = FF_y + F_x$ of (1.1). This is equivalent to the compact representation

$$\rho(E)y_n = h\sigma(E)F_n + h^2\lambda(E)F'_n, \quad E^j y_n = y_{n+j}, \quad (2.2)$$

which shall be loosely depicted as $[\rho, \sigma, \lambda]$ when convenient. Here,

$$\rho(r) = \sum_{j=0}^k \alpha_j r^j, \quad \sigma(r) = \sum_{j=0}^k \beta_j r^j, \quad \lambda(r) = \sum_{j=0}^k \lambda_j r^j,$$

are the associated first, second and third characteristics polynomials of (2.2). The method (2.2) for the numerical solution of the ODEs (1.1) is explicit if $\beta_k = 0$, $\lambda_k = 0$ simultaneously and implicit if atleast one of β_k , λ_k is not zero . It is assumed that the polynomials $\rho(r)$, $\sigma(r)$, $\lambda(r)$ have no common factor. By this (2.1) is said to be an irreducible SDLMM. The instance $\lambda(r) \equiv 0$ is identically zero, then SDLMM (2.2) shall be referred to as a LMM $[\rho(r), \sigma(r)]$, that is $\rho(E)y_n = h\sigma(E)F_n$.

Definition 2.1. A SDLMM (2.2) is said to be of order p ,

$$\begin{aligned}
 \text{if } (a) \quad & \rho(r) - \sigma(r) \log r - \lambda(r) (\log r)^2 = C_{p+1} (r - 1)^{p+1} + O((r - 1)^{p+2}) \\
 \text{or } (b) \quad & \frac{\rho(r)}{\log r} - \sigma(r) - \lambda(r) \log r = C_{p+1} (r - 1)^p + O((r - 1)^{p+1}); \quad C_{p+1} \neq 0 \\
 \text{or } (c) \quad & \frac{\rho(r)}{(\log r)^2} - \frac{\sigma(r)}{\log r} - \lambda(r) = C_{p+1} (r - 1)^{p-1} + O((r - 1)^p)
 \end{aligned}
 \tag{2.3}$$

The C_{p+1} is local truncation error (LTE) constant of the SDLMM (2.1). From (2.3a) or (2.1) we shall have

$$\begin{aligned}
 \rho(e^z) - z\sigma(e^z) - z^2\lambda(e^z) &= \sum_{j=0}^k \alpha_j e^{jz} - z \sum_{j=0}^k \beta_j e^{jz} - z^2 \sum_{j=0}^k \lambda_j e^{jz} \\
 &= C_0 + C_1 z + \dots + C_p z^p + C_{p+1} z^{p+1} + O(z^{p+2}).
 \end{aligned}$$

Thus when the method (2.1) is of order p

$$C_j = 0, \quad C_{p+1} \neq 0; \quad j = 0, 1, \dots, p; \quad p \geq 1$$

Here

$$\left. \begin{aligned}
 C_0 &= \sum_{j=0}^k \alpha_j, \quad C_1 = \sum_{j=0}^k j\alpha_j - \beta_j, \quad C_2 = \sum_{j=0}^k \frac{j^2}{2!} \alpha_j - j\beta_j - \lambda_j, \quad \dots \\
 C_p &= \sum_{j=0}^k \frac{j^p}{p!} \alpha_j - \frac{j^{p-1}}{(p-1)!} \beta_j - \frac{j^{p-2}}{(p-2)!} \lambda_j \quad p \geq 2, \quad k > 1
 \end{aligned} \right\}.$$

Theorem 2.1. The SDLMM $[\rho(r), \sigma(r), \lambda(r)]$ in (2.1) is A-stable, if

$$\begin{aligned}
 \frac{1}{2} \operatorname{Re} \left(\frac{\sigma(r)}{\rho(r)} \pm \sqrt{\left(\frac{\sigma(r)}{\rho(r)} \right)^2 + 4 \frac{\lambda(r)}{\rho(r)}} \right) &> 0, \quad r = \exp^{i\theta}, \\
 i &= \sqrt{-1}, \quad 0 \leq \theta \leq 2\pi
 \end{aligned}
 \tag{2.4}$$

The half is arising from the algebraic process of derivation and can be dropped with no effect on determining A-stability of the SDLMM in (2.2).

Proof. : In the determination of the absolute stability region $R_{AS} = \{z : |r_j(z)| \leq 1; j = 1, 2, \dots, k\}$ where the $r_j(z)$ are the roots of the stability polynomial $\pi(z, r) = \rho(r) - z\sigma(r) - z^2\lambda(r)$ with roots on the unit circle being simple of (2.2) is to have

$$\rho(r) - z\sigma(r) - z^2\lambda(r) = 0, \quad \operatorname{Re}(z) < 0, \quad z = \lambda h \tag{2.5}$$

This is obtained by applying (2.2) on the scalar test problem $y' = \lambda y$, $Re(\lambda) < 0$, the result follows from seeking $\frac{1}{z}$ such that

$$\frac{1}{z^2} - \frac{\sigma(r)}{z\rho(r)} - \frac{\lambda(r)}{\rho(r)} = 0, \tag{2.6}$$

The remainder of the proof follows analogously ([42], page. 247). □

A-stability arises by requiring that $Re\left(\frac{1}{z}\right) > 0$, or $Re(z) > 0$. This is to note that $z \rightarrow \frac{1}{z}$ maps the A-stable region onto itself, with $z = \pm 1$ as the fixed points of this transformation, so that the equivalent requirement

$$Re(z) = \frac{1}{2}Re\left(\frac{\sigma(r)}{\lambda(r)} \pm \sqrt{\left(\frac{\sigma(r)}{\rho(r)}\right)^2 + 4\frac{\lambda(r)}{\rho(r)}}\right) > 0; \tag{2.7}$$

is also valid for A-stability of $[\rho, \sigma, \lambda]$. However, that of (2.4) will be preferred. Note that from (2.6) when $z \rightarrow \infty$, the stability of the SDLMM (2.1) are determined by the roots of $\lambda(r)$ and $\rho(r)$ where $z \rightarrow 0$.

Corollary 2.1. *The SDLMM $[\rho(r), \sigma(r), \lambda(r)]$ in (2.2) is $A(\alpha)$ -stable for some $0 < \alpha < \frac{\pi}{2}$ if*

$$\left| \arg \left[\frac{1}{2} \left(\frac{\sigma(r)}{\lambda(r)} \pm \sqrt{\left(\frac{\sigma(r)}{\rho(r)}\right)^2 + 4\frac{\lambda(r)}{\rho(r)}} \right) \right] - \pi \right| \geq \alpha; \quad r = e^{i\theta},$$

$$i = \sqrt{-1}, \quad 0 \leq \theta \leq 2\pi$$

Proof. : The proof is analogous to ([42], page 252) for LMM. □

This may well pass for the definition of $A(\alpha)$ - stability of a SDLMM. A SDLMM that is stiffly stable is $A(\alpha)$ -stable for some $\alpha < \frac{\pi}{2}$. In fact, for $\alpha = \frac{\pi}{2}$ implies A-stability.

Theorem 2.2. *Let the SDLMM $[\rho(r), \sigma(r), \lambda(r)|k, p]$ be of k -step and of order p with error constant C_{p+1} then,*

$$\frac{-\sigma}{2\lambda} \pm \sqrt{\left(\frac{\sigma^2}{4\lambda^2} + \frac{\rho}{\lambda}\right)} = \log r + \frac{C_{p+1}(r-1)^{p+1}}{\sigma(1)} + O\left((r-1)^{p+2}\right), \quad \sigma(1) \neq 0 \tag{2.8}$$

Proof. : Now the error constant of $[\rho(r), \sigma(r), \lambda(r)]$ is C_{p+1} , so that

$$\rho(r) - z\sigma(r) - z^2\lambda(r) = C_{p+1}(r-1)^{p+1} + O\left((r-1)^{p+2}\right)$$

$$\frac{\rho}{\lambda} - \frac{z\sigma}{\lambda} - z^2 = \frac{C_{p+1}(r-1)^{p+1} + O\left((r-1)^{p+2}\right)}{\lambda}$$

$$z = \frac{-\sigma}{2\lambda} \pm \sqrt{\frac{\sigma^2}{4\lambda^2} + \frac{\rho}{\lambda} - \left(\frac{C_{p+1}(r-1)^{p+1} + O((r-1)^{p+2})}{\lambda} \right)}$$

which by binomial expansion

$$z = \frac{-\sigma}{2\lambda} \pm \sqrt{\frac{\sigma^2}{4\lambda^2} + \frac{\rho}{\lambda}} - \frac{C_{p+1}(r-1)^{p+1} + O((r-1)^{p+2})}{2\lambda(r)\sqrt{\frac{\sigma^2}{4\lambda^2} + \frac{\rho}{\lambda}}}$$

Note that $z = \log r$. Expanding in powers of $r - 1$, where $\rho(1) = 0, \sigma(1) \neq 0, \lambda(1) \neq 0$, then

$$\begin{aligned} \sigma^2(r) + 4\lambda(r)\rho(r) &= \sigma^2(1) + (r-1)(2\sigma(1)r' + 4\lambda(1)\rho'(1)) + \\ &\frac{(r-1)^2}{2} \left(2\sigma'(1)\sigma'(1) + \sigma''(1) + 8\lambda'(1)\rho'(1) + \lambda(1)\rho''(1) \right) \\ &+ O((r-1)^3), \quad |r-1| < 1 \end{aligned}$$

So that

$$\begin{aligned} \sqrt{\sigma^2(r) + 4\lambda(r)\rho(r)} \Big|_{r=1} &= \\ \sigma(1) \left(\sqrt{1 + \frac{(r-1)(2\sigma(1)\sigma'(1) + 4\lambda\rho'(1)) + O((r-1)^2)}{\sigma^2(1)}} \right) &\approx \quad (2.9) \\ \sigma(1) + O(r-1) & \end{aligned}$$

This implies that

$$\frac{-\sigma(r)}{2\lambda(r)} \pm \sqrt{\left(\frac{\sigma(r)}{2\lambda(r)} \right)^2 + \frac{\rho}{\lambda(r)}} = \log r + \frac{C_{p+1}(r-1)^{p+1}}{\sigma(1)} + O((r-1)^{p+2})$$

□

Here $\frac{C_{p+1}}{\sigma(1)}$ is then the normalised error constant of the method in (2.2).

2.1. A Recursive Derivation of Higher Order $A(\alpha)$ -stable SDLMM.

Several notable methods exist for the derivation of SDLMM and in particular, $A(\alpha)$ -stable SDLMM. This section considers an approach of a recursive means of obtaining high order $A(\alpha)$ -stable SDLMM. Here we point to where there is potential to obtain a parametrized $A(\alpha)$ -stable SDLMM from (2.2). The following theorem which is applicable recursively to obtain high order $A(\alpha)$ -stable methods of (2.2) is in this regard.

Theorem 2.3. *Let the SDLMM $[\rho, \sigma, \lambda]$ (2.2) be k -step and $A(\alpha)$ -stable of order p such that*

$$\begin{cases} \rho(1) = 0 \\ \rho(r) \neq 0; \\ \sigma(r) \neq 0, \quad \lambda(r) \neq 0; \end{cases} \quad \begin{cases} |r| = 1, & r \neq 1 \\ |r| = 1 \end{cases} \quad (2.10)$$

then given α_1, α_2 such that $\alpha_1, \alpha_2 < \alpha$ there exist $A(\alpha_1)$, and $A(\alpha_2)$ -stable $(k + 1)$ -step SDLMM (2.2) of order $p + 1$ which also satisfies the requirement of (2.10).

Proof. : The proof which is by constructing the $A(\alpha_1), A(\alpha_2)$ -stable SDLMM, however follows closely a similar one for LMM in ([42], pages. 252 – 253) with the original idea from [50]. Since the SDLMM $[\rho, \sigma, \lambda]$ is of order p with error constant C_{p+1} then

$$\begin{aligned} \rho(r) - \sigma(r) \log r - \lambda(r) (\log r)^2 &= C_{p+1} (r - 1)^{p+1} \\ &+ C_{p+2} (r - 1)^{p+2} + O\left((r - 1)^{p+3}\right), \quad p \geq 2 \end{aligned} \quad (2.11)$$

By this, the two cases in the theorem 2.3 are captured by the following

$$\begin{aligned} \frac{\rho(r)}{\log r} - \sigma(r) - \lambda(r) \log r &= C_{p+1} (r - 1)^p \\ &+ C_{p+2}^{*(1)} (r - 1)^{p+1} + O\left((r - 1)^{p+2}\right) \end{aligned} \quad (2.12)$$

and

$$\begin{aligned} \frac{\rho(r)}{(\log r)^2} - \frac{\sigma(r)}{\log r} - \lambda(r) &= C_{p+1} (r - 1)^{p-1} \\ &+ C_{p+2}^{*(2)} (r - 1)^p + O\left((r - 1)^{p+1}\right) \end{aligned} \quad (2.13)$$

respectively. From the definition in (2.3) of the order p of a SDLMM (2.2). Because of the requirement of zero-stability, we can multiply (2.12) and (2.13) by $(r - 1 + \varepsilon)$ where ε is the parameter such that $0 < \varepsilon < 1$ to obtain the $(k + 1)$ -step two $A(\alpha_i)$ -stable SDLMM $[\widehat{\rho}(r), \widehat{\sigma}_i(r), \widehat{\lambda}_i(r)], i = 1, 2$ of order $p + 1$ defined by

$$\begin{cases} \widehat{\rho}(r) = \rho(r)(r - 1 + \varepsilon) \\ \widehat{\sigma}_1(r) = \sigma(r)(r - 1 + \varepsilon) + \varepsilon C_{p+1} (r - 1)^p \\ \widehat{\lambda}_1(r) = \lambda(r)(r - 1 + \varepsilon); \end{cases} \quad 0 < \varepsilon < 1, \quad (2.14)$$

and the other as

$$\begin{cases} \widehat{\rho}(r) = \rho(r)(r - 1 + \varepsilon) \\ \widehat{\sigma}_2(r) = \sigma(r)(r - 1 + \varepsilon) \\ \widehat{\lambda}_2(r) = \lambda(r)(r - 1 + \varepsilon) + \varepsilon C_{p+1} (r - 1)^{p-1}, \end{cases} \quad 0 < \varepsilon < 1 \quad (2.15)$$

respectively with the polynomials $\widehat{\rho}(r), \widehat{\sigma}_i(r), \widehat{\lambda}_i(r); i = 1, 2$ being of degree at most $k + 1$. It is to be emphasized that we are working with the transformation

$$\frac{1}{z} = \frac{1}{2} \left(\frac{\sigma}{\rho} \pm \sqrt{\left(\frac{\sigma}{\rho}\right)^2 + 4\frac{\lambda}{\rho}} \right)$$

instead of

$$z = \frac{1}{\frac{1}{2} \left(\frac{\sigma}{\rho} \pm \sqrt{\left(\frac{\sigma}{\rho}\right)^2 + 4\frac{\lambda}{\rho}} \right)} \quad \text{or} \quad z = \frac{1}{2} \left(\frac{-\sigma}{\lambda} \pm \sqrt{\left(\frac{\sigma}{\lambda}\right)^2 + 4\frac{\rho}{\lambda}} \right)$$

This is really immaterial as ([42], page. 252) have pointed out since $z \rightarrow \frac{1}{z}$ maps the sector of $A(\alpha)$ -stability onto itself. But this is in an inverse sense with the fixed point at $z = 1, -1$. The requirement in (2.10) entails that the SDLMM $[\rho, \sigma, \lambda|k, p]$ with k -step has $\rho(r)$ with only a root on the unit circle and that root is $r = 1$. It is readily verified that the new SDLMM (2.14) and (2.15) satisfies the requirement in (2.10). It is possible to compare the angles of stability α_1 of (2.14) and α_2 of (2.15) with the original $A(\alpha)$ -stable method $[\rho, \sigma, \lambda]$ which is the generating method from which they have been obtained. This we can do by comparing the boundary-locus of the three SDLMM. Then using (2.14) and (2.15), along with (2.9),

$$\begin{aligned} & \left(\frac{\widehat{\sigma}_i}{\widehat{\rho}_i} \pm \sqrt{\frac{\widehat{\sigma}_i^2}{4\widehat{\rho}_i^2} + \frac{\widehat{\lambda}_i}{\widehat{\rho}_i}} \right) - \left(\frac{\sigma}{2\rho} \pm \sqrt{\frac{\sigma^2}{4\rho^2} + \frac{\lambda}{\rho}} \right) \approx \\ & \begin{cases} \frac{\varepsilon C_{p+1}(r-1)^p}{2\rho(r-1+\varepsilon)} \left(1 \pm \frac{\sigma}{2\rho\sqrt{\frac{\sigma^2}{4\rho^2} + \frac{\lambda}{\rho}}} \right); & i = 1 \\ \frac{\varepsilon C_{p+1}(r-1)^{p-1}}{2\widehat{\rho}\sqrt{\frac{\sigma^2}{4\rho^2} + \frac{\lambda}{\rho}}}; & i = 2 \end{cases} \quad (2.16) \\ & \approx \begin{cases} \frac{\varepsilon C_{p+1}(r-1)^p}{2\rho(r-1+\varepsilon)} \left(1 \pm \frac{\sigma(r)}{\sigma(1)} \right) & i = 1 \\ \frac{\varepsilon C_{p+1}(r-1)^{p-1}}{(r-1+\varepsilon)\sigma(1)}; & i = 2 \end{cases} \end{aligned}$$

and

$$\begin{aligned} & \left(\frac{\widehat{\sigma}_1}{2\widehat{\rho}} \pm \sqrt{\frac{\widehat{\sigma}_1^2}{4\widehat{\rho}^2} + \frac{\widehat{\lambda}_1}{\widehat{\rho}}} \right) - \left(\frac{\widehat{\sigma}_2}{2\widehat{\rho}} \pm \sqrt{\frac{\widehat{\sigma}_2^2}{4\widehat{\rho}^2} + \frac{\widehat{\lambda}_2}{\widehat{\rho}}} \right) \approx \\ & \frac{(r-1)^p}{2\widehat{\rho}} \left[\frac{C_{p+2}^{(2)}}{\sqrt{\frac{\widehat{\sigma}_2^2}{4\widehat{\rho}^2} + \frac{\widehat{\lambda}_2}{\widehat{\rho}}}} - \frac{C_{p+2}^{(2)}}{\sqrt{\frac{\widehat{\sigma}_1^2}{4\widehat{\rho}^2} + \frac{\widehat{\lambda}_1}{\widehat{\rho}}}} \right] \quad (2.17) \\ & \approx (r-1)^p \left(\frac{\varepsilon}{2} \right) \frac{C_{p+1}}{\sigma(1)}; \end{aligned}$$

$$p \geq 2, \quad \widehat{\rho} = \widehat{\rho}_1 = \widehat{\rho}_2$$

where $C_{p+2}^{(1)}, C_{p+2}^{(2)}$ are the error constants of the methods in (2.14) and (2.15) respectively. The (2.16) points to the uniform convergence of the boundary loci of $[\widehat{\rho}_i, \widehat{\sigma}_i, \widehat{\lambda}_i|k+1, p+1], i = 1, 2$ to that of $[\rho, \sigma, \lambda|k, p]$, for a small $\varepsilon > 0$. Similarly (2.17) shows that there may not be any

significant difference between the boundary locus of $[\widehat{\rho}, \widehat{\sigma}_1, \widehat{\lambda}_1|k + 1, p + 1]$, and $[\widehat{\rho}, \widehat{\sigma}_2, \widehat{\lambda}_2|k + 1, p + 1]$, for a very small $\varepsilon(> 0)$. In both cases, the angle between the boundary-loci is of the order $O(\varepsilon)$ as seen from the origin. Define the angle of stability $\alpha_i = \arg\left(\frac{\widehat{\sigma}_i}{\widehat{\rho}_i} \pm \sqrt{\frac{\widehat{\sigma}_i^2}{4\widehat{\rho}_i^2} + \frac{\widehat{\lambda}_i}{\widehat{\rho}_i}}\right)$, $i = 1, 2$ for the recursively derived SDLMM (2.14) and (2.15) respectively. The α is similarly defined for (2.2). By the above $|\alpha_i - \alpha| = O(\varepsilon)$ in (2.16). Moreso, $|\alpha_2 - \alpha_1| = O(\varepsilon)$ from (2.17) accordingly. \square

Now the choice of ε may be guided where it is feasible by the need to minimize functions evaluations, have smaller error constant of the resultant SDLMM or maximise the stability angles α_1, α_2 . The last ensures that the difference in angle of stability $|\alpha - \alpha_1|, |\alpha - \alpha_2|$ or $|\alpha_1 - \alpha_2|$ is minimized. It is observed in general that the angles of stability are such that $\alpha_2 \leq \alpha_1 \leq \alpha$ and if α_3 is the stability angle for a weighted linear combination of (2.14) and (2.15) (to be considered later) then similarly, $\alpha_2 \leq \alpha_3 \leq \alpha_1 \leq \alpha$. The difference in magnitude of any two of these angles is of the $O(\varepsilon)$ in general. This difference becomes divergent on an indefinite re-application of the recursive processes defined by (2.14) and (2.15) with (2.2) as the generating method. In order to obtain a $(k + 1)$ -step SDLMM from the recursive process in (2.14) and (2.15) the order of the generating SDLMM $[\rho, \sigma, \lambda]$ in (2.2) need suitably be $p = k$ or $p = k + 1$ or $p = k + 2$. An example is the second derivative linear multistep methods in [46],

$$y_{n+k} - y_{n+k-1} = h \sum_{j=0}^k \beta_j F_{n+j} + h^2 \gamma_k F'_{n+k}, \quad n = 0, 1, \dots, p = k + 2. \tag{2.18}$$

where the coefficients $\{\beta_j\}_{j=0}^k$ and γ_k are determined so that the maximum order of $p = k + 2$ is attained. The scheme in (2.18) are suitable candidates for the application of theorem (2.3) because of its order $p = k + 2$. The method in (2.18) provides zero-stable methods up to $k = 7$. It is A -stable for $k = 1, 2$, $A(\alpha)$ - stable for $k = 3, 4, 5, 6, 7$ and become zero-unstable methods when $k \geq 8$. The second derivative BDF (SDBDF)

$$\sum_{j=1}^k \left(\sum_{i=j}^k \frac{1}{i} \right) \frac{\nabla^j y_{n+1}}{j} = \left(\sum_{i=1}^k \frac{1}{i} \right) h F_{n+1} - \frac{h^2}{2} F'_{n+1}; \quad k = 1, 2, \dots, 10 \tag{2.19}$$

is also a suitable candidate for the application of theorem (2.3). This method is of order $p = k + 1$. ([42], page 265). It is A -stable for $k = 1, 2, 3$ and $A(\alpha)$ -stable $k = 4, 5, \dots, 10$ and unstable for $k \geq 11$. Theorem (2.3) can be applied recursively on the SDBDF (2.19) to obtain further $A(\alpha)$ - stable SDLMM for some $\alpha < \frac{\pi}{2}$. In particular, for the SDBDF (2.19), the associated characteristics polynomials are

$$\rho(r) = \sum_{j=0}^k \alpha_j r^j, \quad \sigma(r) = \beta_k r^k, \quad \lambda(r) = \lambda_k r^k$$

A first application of the recursion defined by (2.14) and (2.15) gives the recursive SDLMM (RSDLMM)

$$\begin{cases} \widehat{\rho}_1 = \widehat{\rho}(r) = \rho(r)(r - 1 + \varepsilon), & \widehat{\sigma}_1(r) = \beta_k r^k (r - 1 + \varepsilon) + \varepsilon C_{p+1} (r - 1)^{k+1}, \\ \widehat{\lambda}_1(r) = \lambda_k (r - 1 + \varepsilon), \\ \widehat{\rho}_2 = \widehat{\rho}(r), & \widehat{\sigma}_2(r) = \beta_k r^k (r - 1 + \varepsilon), \\ \widehat{\lambda}_2(r) = \lambda_k (r - 1 + \varepsilon) + \varepsilon C_{p+1} (r - 1)^k, & 0 < \varepsilon < 1 \end{cases} \quad (2.20)$$

with $p = k + 2$, as the order of this resultant SDLMM where the respective error constants C_{p+1} of SDLMM of Enright (2.18), SDBDF (2.19), difference corrected SDBDF (2.21) and difference corrected (2.22) are reported in Table 1 for various step number k . The plot of the

TABLE 1. The Error constant C_{p+1} of difference corrected SDBDF in (2.22) and (2.21) with $p = k + 1$.

Step length	Error constant C_{p+1}				
	k	SDLMM of Enright (2.18)	SDBDF (2.19)	SDBDF (2.22)	SDBDF (2.21)
1		$\frac{1}{7}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{8}$
2		$\frac{-1}{180}$	$\frac{1}{21}$	$\frac{1}{9}$	$\frac{1}{18}$
3		$\frac{-11}{7200}$	$\frac{9}{425}$	$\frac{1}{16}$	$\frac{1}{32}$
4		$\frac{1}{1512}$	$\frac{24}{2075}$	$\frac{1}{25}$	$\frac{1}{50}$
5		$\frac{191}{846720}$	$\frac{600}{84133}$	$\frac{1}{36}$	$\frac{1}{72}$
6		$\frac{-23}{226800}$	$\frac{450}{94423}$	$\frac{1}{49}$	$\frac{1}{98}$
7		$\frac{-2497}{65318400}$	$\frac{3600}{726301}$	$\frac{1}{64}$	$\frac{1}{128}$
8		$\frac{263}{1496800}$	$\frac{2450}{726301}$	$\frac{1}{81}$	$\frac{1}{162}$
9		$\frac{14797}{2107607400}$	$\frac{7840}{3144919}$	$\frac{1}{100}$	$\frac{1}{200}$
10		$\frac{-133787}{40864824000}$	$\frac{529200}{353764433}$	$\frac{1}{121}$	$\frac{1}{242}$

Note: the SDBDF in (2.22) has the error constant $C_{p+1} = \frac{1}{(k+1)^2}$ and similarly, the error constant of SDBDF in (2.21) is $C_{p+1} = \frac{1}{2(k+1)^2}$

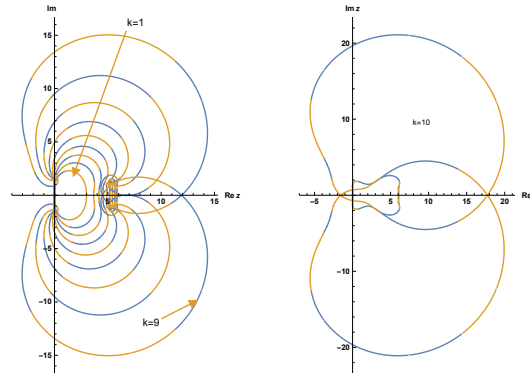


FIGURE 1. Stability region (exterior of closed curves) of difference corrected SDBDF (2.21) for $k = 1, 2, \dots, 9$ and stability interval for $k = 10$ is $(-1.2, 0]$.

stable methods for $\varepsilon = \frac{1}{2}$ and $k = 1, 2, \dots, 8$ in the first and $k = 1, 2, \dots, 5$ in the second methods in (2.20) are given in Fig 2b, 3a respectively. When we put $h \nabla^k F_{n+1}$ for $\nabla^{k+1} y_{n+1}$, the relation (2.19) therefore suggest the difference corrected SDBDF

$$\sum_{j=1}^k \left(\sum_{i=j}^{k+1} \frac{1}{i} \right) \frac{\nabla^j y_{n+1}}{j} = h \left(\left(\sum_{i=1}^{k+1} \frac{1}{i} \right) F_{n+1} - \frac{1}{k+1} \frac{\nabla^k F_{n+1}}{k+1} \right) - \frac{h^2}{2} F'_{n+1} \quad (2.21)$$

is of order $p = k + 1$. It is zero-stable for $k = 1, 2, \dots, 13$, A -stable for $k = 1, 2, 3$ and $A(\alpha)$ -stable $k = 4, 5, \dots, 9$ and unstable for $k \geq 14$ (see Fig. 1 for the stability boundary loci plot). Another difference corrected SDBDF of the same order is obtained when we put $h^2 \nabla^{k-1} F'_{n+1}$ for $\nabla^{k+1} y_{n+1}$,

$$\sum_{j=1}^k \left(\sum_{i=j}^{k+1} \frac{1}{i} \right) \frac{\nabla^j y_{n+1}}{j} = h \left(\sum_{i=1}^{k+1} \frac{1}{i} \right) F_{n+1} - \frac{h^2}{2} \left(F'_{n+1} + \frac{2}{k+1} \frac{\nabla^{k-1} F'_{n+1}}{k+1} \right); \quad p = k+1. \quad (2.22)$$

Similarly, this method is A -stable for $k = 1, 2, 3$ and $A(\alpha)$ -stable $k = 4, 5, \dots, 14$ as shown in Fig. 4.

However, we are unable to obtain the stability plot for step number $k \geq 15$ in the difference corrected SDBDF (2.22) due to computational limitation of our computing device. These are further candidates for recursive derivation of $A(\alpha)$ -stable SDLMM from theorem (2.3) using (2.14) and (2.15) accordingly. One obtains SDLMM (2.1) with future points when we apply (2.14) and (2.15) to a generating second derivative linear method with order $p \geq k + 3$ and step length k .

Theorem 2.4. Suppose $[\rho, \sigma, \lambda|k, p]$ is $A(\alpha)$ -stable. Let $[\rho_1, \sigma_1, \lambda_1|k+1, p+1]$, and $[\rho_2, \sigma_2, \lambda_2|k+1, p+1]$, be the associated $A(\alpha_1)$, $A(\alpha_2)$ -stable SDLMM generated from $[\rho, \sigma, \lambda|k, p]$ in (2.14)

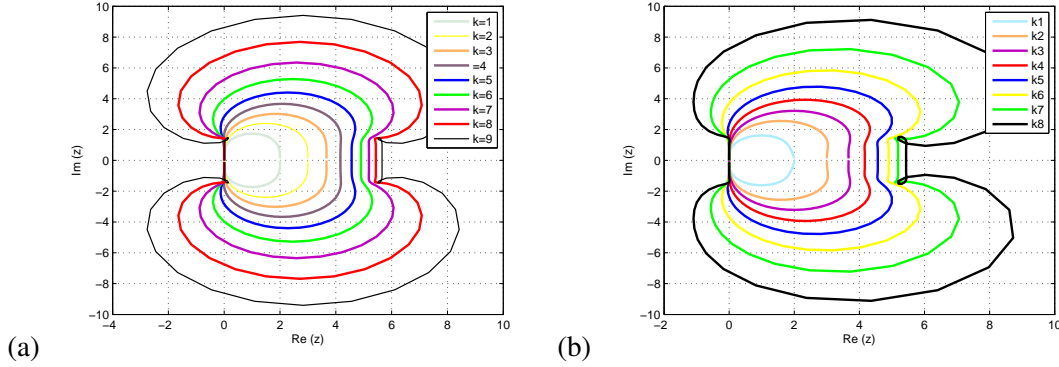


FIGURE 2. (a)–Stability region (exterior of closed curves) of SDBDF (2.19) and (b)– RSDBDF from (2.14) ($\varepsilon = \frac{1}{2}$).

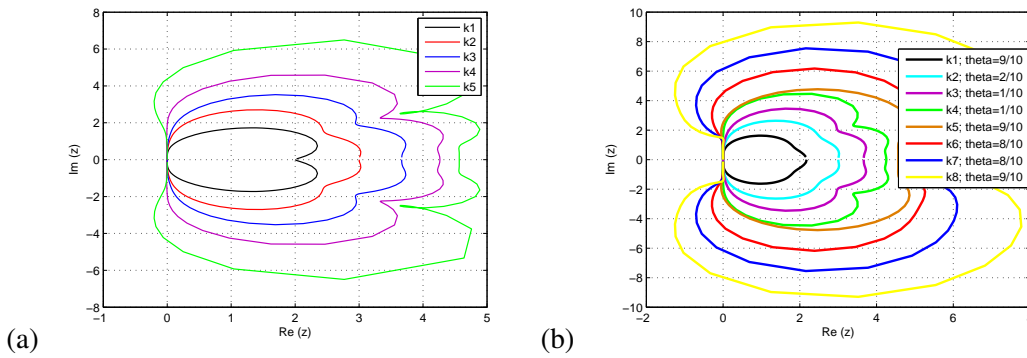


FIGURE 3. (a)– Stability region (exterior of closed curves) of RSDBDF from (2.15) ($\varepsilon = \frac{1}{2}$) and (b)–Weighted linear combination (2.27) for various θ .

and (2.15) respectively, with $\rho_1(r) = \rho_2(r)$. Then

$$C_{p+2}^{(1)} = C_{p+1} + \varepsilon \left(C_{p+2} + \frac{1}{2}C_{p+1} \right), \quad \frac{C_{p+2}^{(1)}}{\widehat{\sigma}_1(1)} \tag{2.23}$$

$$C_{p+2}^{(2)} = C_{p+1} + \varepsilon (C_{p+2} + C_{p+1}), \quad \frac{C_{p+2}^{(2)}}{\widehat{\sigma}_2(1)} \tag{2.24}$$

$$\widehat{\sigma}_i(1) = \sigma(1)\varepsilon, i = 1, 2; \sigma(1) \neq 0$$

are the error and the normalized error constants of (2.14) and (2.15) respectively. Notice that $C_{p+2}^{(2)} - C_{p+2}^{(1)} = \frac{1}{2}C_{p+1}$, implying of course that (2.14) has a smaller error constant than that from (2.15).

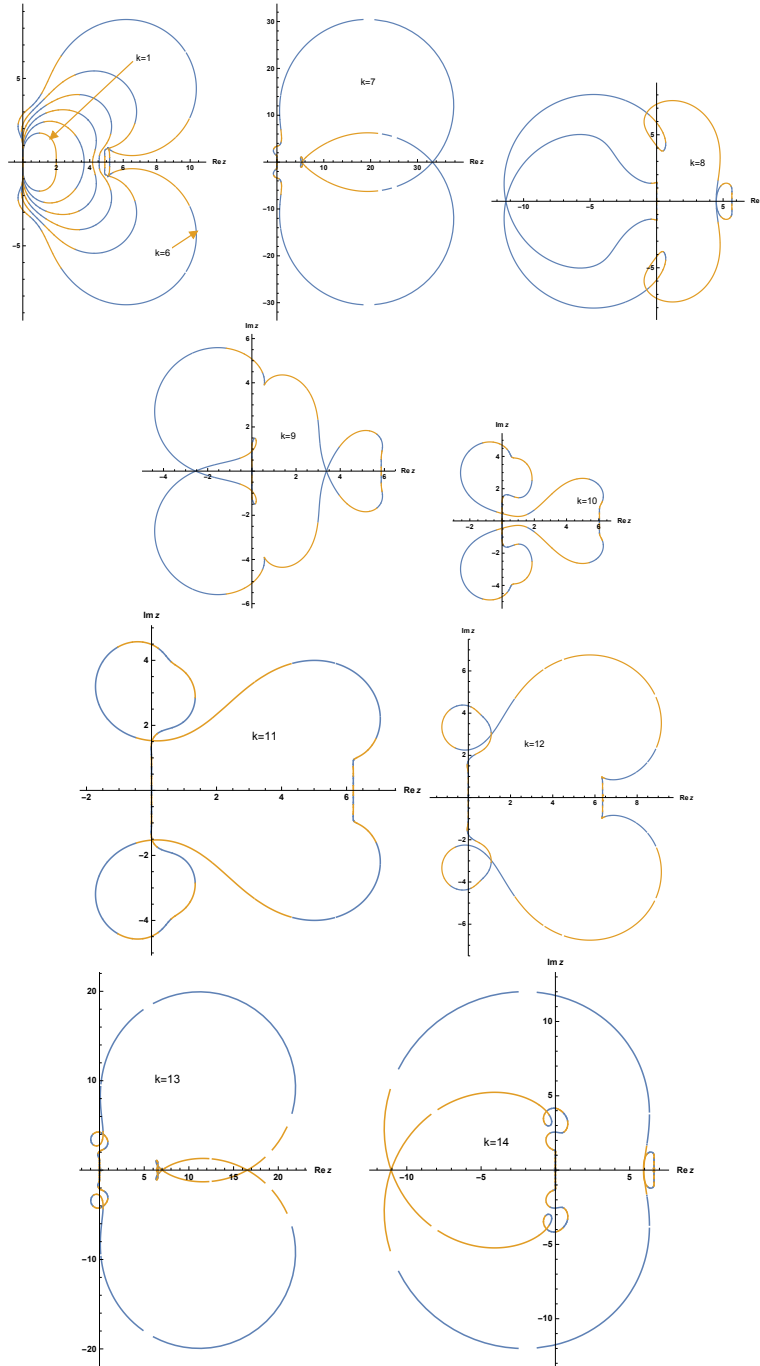


FIGURE 4. Stability region (exterior of closed curves) of difference corrected SDBDF (2.22) for $k = 1, 2, \dots, 7, 10, 11, 12, 13$. For the case of $k = 8$ and 14 , the interval of stability is $(-11, 0]$, $k = 9$, $(-2, 0]$

Proof. : Since

$$\begin{aligned} \rho(r) - \sigma(r) \log r - (\log r)^2 \lambda(r) &= C_{p+1} (r-1)^{p+1} + C_{p+2} (r-1)^{p+2} \\ &\quad + C_{p+3} (r-1)^{p+3} + O((r-1)^{p+4}) \end{aligned}$$

Now,

$$\frac{1}{\log r} = \frac{1}{r-1} + \frac{1}{2} - \frac{r-1}{12} + \frac{(r-1)^2}{24} - \frac{19(r-1)^3}{720} + \dots, \quad z = \log r$$

Thus $\left(\frac{1}{\log r}\right)^2$ can be obtained readily. Thus for (2.14),

$$\begin{aligned} &\frac{\rho(r)(r-1+\varepsilon)}{\log r} - \sigma(r)(r-1+\varepsilon) - \lambda(r)(r-1+\varepsilon) \log r \\ &= (r-1+\varepsilon) \left(\frac{C_{p+1} (r-1)^{p+1} + C_{p+2} (r-1)^{p+2} + O((r-1)^{p+3})}{\log r} \right), \\ &\quad \frac{\rho(r)(r-1+\varepsilon)}{\log r} - \sigma(r)(r-1+\varepsilon) - \varepsilon C_{p+1} (r-1)^p \\ &\quad - \lambda(r)(r-1+\varepsilon) \log r = \left[C_{p+1} + \varepsilon \left(C_{p+2} + \frac{1}{2} C_{p+1} \right) \right] (r-1)^{p+1} \quad (2.25) \\ &\quad + \left(C_{p+3} + \frac{1}{2} C_{p+2} - \frac{1}{12} C_{p+1} \right) (r-1)^{p+2} + O((r-1)^{p+3}) \end{aligned}$$

That of (2.15) is given by

$$\begin{aligned} &\frac{\rho(r)(r-1+\varepsilon)}{(\log r)^2} - \frac{\sigma(r)(r-1+\varepsilon)}{\log r} - \lambda(r)(r-1+\varepsilon) \\ &= [C_{p+1} (r-1)^{p+1} + O((r-1)^{p+2})] (r-1+\varepsilon) \left(\frac{1}{\log r} \right)^2 \\ &\quad \frac{\rho(r)(r-1+\varepsilon)}{(\log r)^2} - \frac{\sigma(r)(r-1+\varepsilon)}{\log r} - \lambda(r)(r-1+\varepsilon) \\ &\quad - \varepsilon C_{p+1} (r-1)^{p-1} = [C_{p+1} + \varepsilon (C_{p+2} + C_{p+1})] (r-1)^p \quad (2.26) \\ &\quad + \left(C_{p+3} + C_{p+2} - \frac{1}{12} C_{p+1} \right) (r-1)^{p+1} + O((r-1)^{p+2}) \end{aligned}$$

The results follow directly from the first coefficient of the expansion in (2.25) and (2.26). \square

The SDLMM (2.14) has smaller error constant than that from (2.15). Thus (2.14) is expected to have better accuracy and linear stability characteristics than the method of (2.15), since they are of the same order of convergence. This is the case practically as Fig.2b, 3a will show. Further $A(\alpha)$ -stable methods can be obtained by a weighted linear combination of

$[\rho_i(r), \sigma_i(r), \lambda_i(r) | k + 1, p + 1]$, $i = 1, 2$ from (2.14) and (2.15) accordingly in the following sense. Multiply (2.14) by θ and (2.15) by $(1 - \theta)$ to obtain the resultant SDLMM,

$$\begin{aligned} \rho(r)(r - 1 + \varepsilon) &= h [\sigma(r)(r - 1 + \varepsilon) + \theta \varepsilon C_{p+1}(r - 1)^p] \\ &+ h^2 [\lambda(r)(r - 1 + \varepsilon) + (1 - \theta) \varepsilon C_{p+1}(r - 1)^{p-1}]; \quad 0 \leq \theta \leq 1 \end{aligned} \tag{2.27}$$

When we do the same, but with θ and $(1 - \theta)$ interchanged then,

$$\begin{aligned} \rho(r)(r - 1 + \varepsilon) &= h [\sigma(r)(r - 1 + \varepsilon) + (1 - \theta) \varepsilon C_{p+1}(r - 1)^p] \\ &+ h^2 [\lambda(r)(r - 1 + \varepsilon) + \theta \varepsilon C_{p+1}(r - 1)^{p-1}]; \quad 0 \leq \theta \leq 1 \end{aligned} \tag{2.28}$$

The resultant methods are certainly not the same when $\theta \neq \frac{1}{2}$. A particular example is the linear combination

$$\sum_{j=1}^k \left(\sum_{i=j}^{k+1} \frac{1}{i} \right) \frac{\nabla^j y_{n+1}}{j} = h \left(\sum_{i=1}^{k+1} \frac{1}{i} \right) F_{n+1} - \frac{h^2}{2} F'_{n+1} - \begin{cases} h \frac{\theta}{k+1} \frac{\nabla^k F_{n+1}}{k+1} + h^2 \frac{(1-\theta)}{k+1} \frac{\nabla^{k-1} F'_{n+1}}{k+1} \\ h \frac{(1-\theta)}{k+1} \frac{\nabla^k F_{n+1}}{k+1} + h^2 \frac{\theta}{k+1} \frac{\nabla^{k-1} F'_{n+1}}{k+1} \end{cases}$$

of the difference corrected methods in (2.21) and (2.22).

Theorem 2.5. *The error constants of the SDLMM in (2.27) and (2.28) are given by*

$$\begin{cases} C_{p+1}^{*(1)} = C_{p+1} + \varepsilon (C_{p+2} + (1 - \frac{\theta}{2}) C_{p+1}) \\ C_{p+1}^{*(2)} = C_{p+1} + \varepsilon (C_{p+2} + (\frac{1+\theta}{2}) C_{p+1}) \end{cases}$$

respectively. *Moreso*, $C_{p+1}^{*(1)} - C_{p+1}^{*(2)} = (\frac{1}{2} - \theta) C_{p+1}$

Proof. : The proof is analogous to that of theorem (2.4). □

We can now prove following [42], the following result for SDLMM

Theorem 2.6. *Suppose that $\alpha \leq \frac{\pi}{2}$ is given. Then for every $k \in N^+$, there exist two $A(\alpha_i)$ -stable ($i = 1, 2$) k -step SDLMM $[\rho_i, \sigma_i, \lambda_i]$, $i = 1, 2$ each of order $p = k + 1$ but with different error constants given by (2.23) and (2.24).*

Proof. : The proof follows same line of reasoning on page 252 in [42]
In particular for $k = 1, p = 2$ the one-step SDBDF (2.19) which is A -stable is therefore $A(\alpha_i^{(2)})$ -stable for every $\alpha_i^{(2)} \leq \frac{\pi}{2}$. For an arbitrary $k \in N^+$, we can following [42] intercalate $k - 2$ values of two sequences between α_i , and $\frac{\pi}{2}$, that is,

$$\alpha_i^{(k)} = \alpha_i < \alpha_i^{(k-1)} < \dots < \alpha_i^{(2)} \leq \frac{\pi}{2} = \alpha_i^{(1)}, \quad i = 1, 2$$

and extend the methods from step number-to-step number by theorem (2.3). The error constants are given by theorem (2.4) □

Theorem 2.7. *If a SDLMM $[\rho, \sigma, -\lambda|p, k]$ in the convention of (2.2) (i.e $\rho(E)y_n = h\sigma(E)F_n - h^2\lambda(E)F'_n$) is A-stable then*

$$\begin{cases} (a) & \operatorname{Re}\left(\frac{\sigma}{\rho}\right) > 0, \quad \operatorname{Re}\left(\frac{\lambda}{\sigma}\right) > 0 \\ (b) & \operatorname{Re}\left(\frac{\sigma}{\rho}\right) > 0, \quad \operatorname{Re}\left(\left(\left(\frac{\sigma}{\rho}\right)^{\frac{1}{2}} - \left(\frac{\sigma}{\rho} - 4\frac{\lambda}{\sigma}\right)^{\frac{1}{2}}\right)^2\right) > 0 \end{cases}$$

The first (a) is a necessary condition and the second (b) is sufficient for the A-stability of $[\rho, \sigma, \lambda]$.

Proof. : The proof of the first is by contradiction. In determining linear stability of $[\rho, \sigma, -\lambda]$,

$$\rho(r) - z\sigma(r) + z^2\lambda(r) = 0, \tag{2.29}$$

So that by A-stability, the second result (b) is obtained by restructuring the real part of the root of (2.29),

$$\begin{aligned} \operatorname{Re}\left(\frac{1}{z}\right) &= \frac{1}{2}\operatorname{Re}\left(\frac{\sigma}{\rho} \pm \sqrt{\left(\frac{\sigma}{\rho}\right)^2 - 4\frac{\lambda}{\rho}}\right) = \\ &\frac{1}{2}\operatorname{Re}\left(\frac{\sigma}{\rho}\right)^{\frac{1}{2}}\left(\left(\left(\frac{\sigma}{\rho}\right)^{\frac{1}{2}} \pm \left(\frac{\sigma}{\rho} - 4\frac{\lambda}{\sigma}\right)^{\frac{1}{2}}\right)^2\right)^{\frac{1}{2}} > 0 \end{aligned} \tag{2.30}$$

$$\operatorname{Re}(z) = \frac{1}{2}\operatorname{Re}\left(\frac{\sigma}{\lambda} \pm \sqrt{\left(\frac{\sigma}{\lambda}\right)^2 - 4\frac{\rho}{\lambda}}\right) > 0 \tag{2.31}$$

Proving the first (a) is slightly more technical. Suppose otherwise, that is

$$\operatorname{Re}\left(\frac{\sigma(r)}{\rho(r)}\right) < 0 \tag{2.32}$$

and that the method is A-stable, then consider the equation (2.29), for A-stability of the SDLMM $[\rho(r), \sigma(r), -\lambda(r)]$, by theorem (2.1),

$$\operatorname{Re}\left(\frac{\sigma}{\rho} \pm \sqrt{\left(\frac{\sigma}{\rho}\right)^2 - 4\frac{\lambda}{\rho}}\right) = \operatorname{Re}\left(\frac{\sigma}{\rho}\right) \pm \operatorname{Re}\left(\sqrt{\left(\frac{\sigma}{\rho}\right)^2 - 4\frac{\lambda}{\rho}}\right) > 0 \tag{2.33}$$

Then by (2.32) there is a complex root of (2.29) for which its real part in (2.33) is negative, but this contradicts the requirement of A-stability. It is therefore necessary that $\operatorname{Re}\left(\frac{\sigma(r)}{\rho(r)}\right) > 0$, i.e $\operatorname{Re}(z) > 0$ for A-stability of $[\rho(r), \sigma(r), -\lambda(r)]$ and (2.30) is sufficient to attain it. The second part of (a) is proved by similar argument applied on (2.31). \square

We find applications for the above theorem (2.7) in what now follows. They can be proved by direct verification.

Corollary 2.2. A SDBDF (2.19), $\rho(E)y_n = h\beta_k F_{n+k} - h^2\lambda_k F'_{n+k}$; $\lambda_k, \beta_k > 0$ that is $A(\alpha)$ -stable for some $\alpha < \frac{\pi}{2}$ is such that

$$\left| \arg \left(\frac{\beta_k r^k}{\rho(r)} \right) - \pi \right| \geq \gamma, \quad \gamma < \frac{\pi}{2}$$

This is the case for the SDBDF (2.19) for $k \leq 9$.

A SDLMM $[\rho(r), \sigma(r), \lambda(r)]$ of order p , can be constructed given any two of the characteristic polynomials ρ, σ, λ of degree k . To do this,

$$\left(\frac{r^2}{(\log(1+r))^2} \right) \left(\frac{\rho(1+r)}{r^2} \right) + \left(\frac{r}{\log(1+r)} \right) \left(\frac{\sigma(1+r)}{r} \right) - \lambda(1+r) = O(r^p)$$

Thus, if $\rho(r)$ and $\lambda(r)$ are given then,

$$\sigma(1+r) = \frac{\log(1+r)}{\lambda(1+r)} \log(1+r) - \frac{1}{\log(1+r)} \rho(1+r)$$

Corollary 2.3. A SDBDF (2.19), $\rho(E)y_n = h\beta_k F_{n+k} - h^2\lambda_k F'_{n+k}$; $\lambda_k, \beta_k > 0$ that is A -stable is such that

$$\operatorname{Re} \left(\frac{\beta_k r^k}{\rho(r)} \right) > 0$$

and for the SDBDF (2.19), $k \leq 3$.

Theorem 2.8. Suppose that $\rho(E)y_n = h\sigma(E)F_n$ is A -stable k -step LMM $[\rho(r), \sigma(r)]$ of order p . Let it be possible to find $\lambda(r)$ such that $\rho(E)y_n = h\sigma(E)F_n - h^2\lambda(E)F'_n$, $\lambda_k, \beta_k > 0$ is of order p^* and this SDLMM $[\rho(r), \sigma(r), -\lambda(r)]$ is also A -stable. Then

$$\operatorname{Re} \left(\frac{\lambda(r)}{\sigma(r)} \right) > 0.$$

Examples: The methods

$$\begin{cases} y_{n+1} = y_n + hF_{n+1}; & p = 1, & C_2 = \frac{1}{2} \\ y_{n+1} = y_n + hF_{n+1} - \frac{h^2 F'_{n+1}}{2}; & p = 2, & C_3 = \frac{1}{6} \end{cases}$$

$$\begin{cases} y_{n+1} = y_n + \frac{h}{2}[F_n + F_{n+1}], & p = 2, & C_3 = \frac{1}{12} \\ y_{n+1} = y_n + \frac{h}{2}[F_n + F_{n+1}] - \frac{h^2}{12}[-F'_n + F'_{n+1}], & p = 4, & C_5 = \frac{1}{720} \end{cases}$$

which are A -stable are applications of this theorem.

In the circumstance for $A(\alpha)$ -stable methods, theorem (2.8) reduces to what now follows

Theorem 2.9. Suppose that $[\rho(r), \sigma(r)]$ is $A(\alpha_1)$ -stable k -step LMM of order p with the error constant C_{p+1} . Let it be possible to find $\lambda(r)$ such that the SDLMM $\rho(E)y_n = h\sigma(E)F_n - h^2\lambda(E)F'_n$, $\beta_k, \lambda_k > 0$ is of order p^* with error constant $C_{p^*+1}^*$ and the SDLMM $[\rho(r), \sigma(r), -\lambda(r)]$ is also $A(\alpha_2)$ -stable then

$$\left| \arg \left(\frac{\lambda(r)}{\sigma(r)} \right) - \pi \right| \geq \gamma, \quad \gamma \leq \frac{\pi}{2} \tag{2.34}$$

and

$$\frac{1}{2} \left(\frac{\sigma}{\rho} \pm \sqrt{\left(\frac{\sigma}{\rho}\right)^2 - 4\frac{\lambda}{\rho}} \right) = \begin{cases} \frac{C_{p+1}(r-1)^{p^*-1}}{\rho\sqrt{\left(\frac{\sigma}{\rho}\right)^2 - 4\frac{\lambda}{\rho}}}, & p^* - 1 < p \\ (r-1)^p \left(\frac{C_{p^*+1}}{\rho\sqrt{\left(\frac{\sigma}{\rho}\right)^2 - 4\frac{\lambda}{\rho}}} - \frac{C_{p+1}}{\rho} \right), & p^* - 1 = p \\ -\frac{(r-1)^p C_{p+1}}{\rho}, & p^* - 1 > p \end{cases} \quad (2.35)$$

With respect to this theorem, suppose the SDLMM is A-stable then $Re\left(\frac{\lambda}{\sigma}\right) > 0$, $Re\left(\frac{\sigma(r)}{\rho(r)}\right) > 0$, $Re(z) > 0$ by theorem (2.7). By this

$$\left| arg\left(\frac{\lambda(r)}{\sigma(r)}\right) - \pi \right| \geq \frac{\pi}{2}, \quad \left| arg\left(\frac{\sigma(r)}{\rho(r)}\right) - \pi \right| \geq \frac{\pi}{2}$$

Then $A(\alpha)$ -stability of the SDLMM $[\rho(r), \sigma(r), -\lambda(r)]$ imply the existence of $\alpha_1 = \alpha_2$ such that (2.34) holds for some $\gamma \leq \frac{\pi}{2}$. The (2.35) is proved following (2.16) with respect to $[\rho(r), \sigma(r)]$ and $[\rho(r), \sigma(r), -\lambda(r)]$

2.2. Recursive Derivation of LMM. A LMM and a SDLMM can be derived from any of the following means of undetermined coefficients, differentiation, integration, complex variable methods, interpolation and collocation, blended method (weighted linear combination of methods), exponential fitting of LMM in [47]. However, (2.14) and (2.15) serves a simple means of deriving $A(\alpha)$ -stable SDLMM recursively. A similar means is found in ([42], page 252) for the case of LMM $[\rho(r), \sigma(r)]$.

Theorem 2.10. Let $[\rho(r), \sigma(r)]$ be an A-stable k -step LMM ($\lambda(r) \equiv 0$ in (2.1)) of order p such that $\varepsilon C_{p+1} > 0$ then the LMM $[\hat{\rho}(r), \hat{\sigma}(r)]$ defined by

$$\hat{\rho} = \rho(r)(r - 1 + \varepsilon), \quad \hat{\sigma} = \sigma(r)(r - 1 + \varepsilon) + \varepsilon C_{p+1}(r - 1)^p \quad (2.36)$$

is an A-stable $(k + 1)$ -step LMM of order $p + 1$ if,

$$Re\left(\frac{(r - 1)^p}{\rho(r)(r - 1 + \varepsilon)}\right) > 0; \quad r = e^{i\theta}, \quad 0 < \varepsilon < 1, 0 \leq \theta \leq 2\pi$$

By Dahlquist order barrier the restriction is to $k = 1, 2$ with respect to the LMM $[\rho, \sigma]$ with C_{p+1} as its error constant.

The proof of this is rather straight forward. In fact, the error constant of $[\hat{\rho}, \hat{\sigma}]$ is $\hat{C}_{p+2} = C_{p+1} + \varepsilon\left(C_{p+2} + \frac{C_{p+1}}{2}\right)$, where (2.36) have been obtained from

$$\rho(r) - \sigma(r) \log(r) = C_{p+1}(r - 1)^{p+1} + C_{p+2}(r - 1) + O\left((r - 1)^{p+3}\right)$$

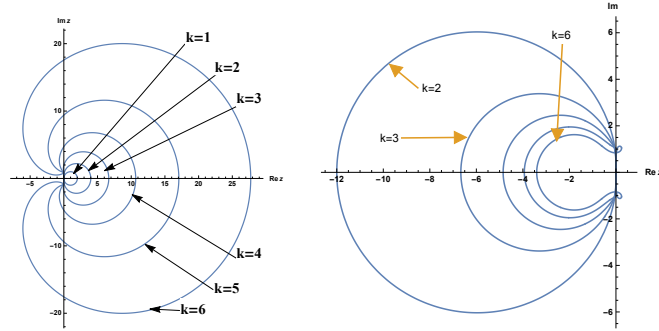


FIGURE 5. (a):Boundary loci of the BDF (2.37) of order $p = k$ and (b): the difference corrected BDF (2.38) of order $p = k + 1$.

following the process leading to (2.14). The relation (2.36) for the LMM $[\rho, \sigma]$ have been obtained in ([42], page 252), which (2.14) and (2.15) are the equivalent for SDLMM $[\rho, \sigma, \lambda]$ in (2.2). The BDF are worthy candidates for obtaining high order $A(\alpha)$ -stable LMM by (2.36),

$$\sum_{j=1}^k \frac{\nabla^j}{j} y_{n+1} = h F_{n+1}; \quad k = 1, \dots, 6, \quad p = k, \tag{2.37}$$

So is the difference corrected BDF, $(\nabla^{k+1} y_{n+1} \rightarrow h \nabla^k F_{n+1})$

$$\sum_{j=1}^k \frac{\nabla^j}{j} y_{n+1} = h \left(F_{n+1} - \frac{\nabla^k}{k+1} F_{n+1} \right); \quad p = k + 1; \tag{2.38}$$

The method in (2.38) is zero stable for the cases of $k = 1, \dots, 16$ as shown in Fig. 5b, where $k = 1$ is the A -stable Trapezoidal rule. The stability interval and error constants of the difference corrected BDF (2.38) for step number k is reported in Table 2, along with the error constants C_{p+1} for the BDF (2.37).

Theorem 2.11. (a)- *Let the recursive relation in (2.36) be applied j number of times on the generating k -step LMM $[\rho, \sigma]$ with error constant C_{p+1} and having the order p . Let the recursively obtained LMM be $[\rho^{[j]}, \sigma^{[j]}]$ with error constant $C^{(j)} = C_{p+j+1}^{(j)}$ and order $p + j$, (in the case of BDF $p = k$) then*

$$\left| \frac{\sigma^{[j]}}{\rho^{[j]}} - \frac{\sigma}{\rho} \right| \leq \frac{2^{p-1} C_*}{\phi_{min}} \left(\frac{1 - (\frac{2}{\varepsilon})^j}{1 - (\frac{2}{\varepsilon})} \right) \leq \frac{\varepsilon C_* 2^{p-2}}{\min_{\theta} |\phi(r)|} \left(\frac{2}{\varepsilon} \right)^j; \quad r = e^{i\theta},$$

$$0 \leq \theta \leq \frac{\pi}{2}, \quad C_* = \max_{0 \leq j_1 \leq j} \left\{ \left| C^{(j_1)} \right| \right\} < \infty, \quad \phi_{min} = \min_{\theta} |\phi(r)|$$

$$\rho(r) = (r - 1)\phi(r)$$

(b)- Let the recursive relation in (2.14) be applied j number of times on the generating k -step SDLMM $[\rho(r), \sigma(r), \lambda(r)]$ with error constant C_{p+1} and having the order p . Let the recursively obtained SDLMM be $[\rho^{[j]}, \sigma^{[j]}, \lambda^{[j]}]$ with error constant $C^{(j)} = C_{p+j+1}^{(j)}$ and order $p + j$, (in

TABLE 2. The stability interval of the difference corrected BDF (2.38) for step length $k = 1, \dots, 16$ with $p = k + 1$.

Error constant C_{p+1} BDF (2.37)	Step number k	Interval of stability region difference corrected BDF (2.38)	Error constant C_{p+1} BDF (2.38)
$-\frac{1}{3}$	2	$(-12.0, 0]$	$-\frac{1}{12}$
$-\frac{1}{4}$	3	$(-6.8, 0]$	$-\frac{3}{40}$
$-\frac{1}{5}$	4	$(-4.9, 0]$	$-\frac{1}{15}$
$-\frac{1}{6}$	5	$(-4.0, 0]$	$-\frac{5}{84}$
$-\frac{1}{7}$	6	$(-3.45, 0]$	$-\frac{3}{56}$
-	7	$(-3.05, -0.4) \cup (-0.4, 0]$	$-\frac{7}{144}$
-	8	$(-2.82, 0]$	$-\frac{2}{45}$
-	9	$(-2.68, 0]$	$-\frac{9}{220}$
-	10	$(-2.58, 0]$	$-\frac{5}{132}$
-	11	$(-2.5, 0]$	$-\frac{11}{312}$
-	12	$(-2.42, 0]$	$-\frac{3}{91}$
-	13	$(-2.4, 0]$	$-\frac{13}{420}$
-	14	$(-2.34, 0]$	$-\frac{7}{240}$
-	15	$(-2.21, 0]$	$-\frac{15}{544}$
-	16	$(-2.19, 0]$	$-\frac{4}{153}$

Note: the BDF in (2.37) has the error constant $C_{p+1} = \frac{1}{k+1}$.

where $\rho(r) = (r - 1)\phi(r)$; $\rho^{j-1}(r) = \rho(r)(r - 1 + \varepsilon)^{j-1}$,

$$|r - 1 + \varepsilon| > |r| - |\varepsilon - 1| = 1 - |\varepsilon - 1| > \varepsilon$$

$$\frac{1}{|\rho^{[j-1]}|} = \frac{1}{|\rho||r - 1 + \varepsilon|^{j-1}} \leq \frac{1}{|\rho|\varepsilon^{j-1}}$$

The (b) part is proof analogously. the same result obtains with (2.15). A consequence of this theorem is captured in what follows. It points to the fact that the generated LMM $\rho^{[j-1]}, \sigma^{[j-1]}$ have deteriorating stability angles $\alpha^{(j)}$ with an indefinite number j of times of application of the recursive processes (2.35) and (2.36). \square

Theorem 2.12. (a)- *The difference in angle of stability between $[\rho^{[j]}, \sigma^{[j]}]$ and $[\rho, \sigma]$ as seen from the origin increases with j as indicated in*

$$\left| \arg \left(\frac{\sigma^{[j]}}{\rho^{[j]}} \right) - \arg \left(\frac{\sigma}{\rho} \right) \right| = O \left(2^{p-2} \left(\frac{2}{\varepsilon} \right)^j \varepsilon \right) = \begin{cases} O(2^{p-1}); & p \geq 2, \quad j = 1 \\ O\left(\left(\frac{2}{\varepsilon}\right)^{j+1} \varepsilon^2\right); & p \geq 3, \quad j \geq 1 \\ O\left(\left(\frac{2}{\varepsilon}\right)^{p+j-2} \varepsilon^{p-1}\right); & p \geq 2, \quad j \geq 1 \end{cases} \tag{2.39}$$

(b)- *The difference in angle of stability between $[\rho^{[j]}, \sigma^{[j]}, \lambda^{[j]}]$ and $[\rho, \sigma, \lambda]$ as seen from the origin increases with j as indicated in*

$$\left| \arg \left(\frac{\hat{\sigma}_1^{[j]} \pm \sqrt{\frac{\hat{\sigma}_1^{[j]}}{2\hat{\rho}_1^{[j]} + \frac{\hat{\lambda}_1^{[j]}}{\hat{\rho}_1^{[j]}}}}}{\hat{\rho}_1^{[j]}} \right) - \arg \left(\frac{\sigma}{2\rho} \pm \sqrt{\frac{\sigma^2}{4\rho^2} + \frac{\lambda}{\rho}} \right) \right|$$

$$= O \left(2^{p-2} \left(\frac{2}{\varepsilon} \right)^{j-1} \right) = \begin{cases} O(2^{p-2}); & p \geq 2, \quad j = 1 \\ O\left(2 \left(\frac{2}{\varepsilon}\right)^{j-1}\right); & p \geq 3, \quad j \geq 1 \\ O\left(\left(\frac{2}{\varepsilon}\right)^{p+j-3} \varepsilon^{p-2}\right); & p \geq 2, \quad j \geq 1 \end{cases} \tag{2.40}$$

The j is the number of times of re-application of the recursions defined by (2.14) and (2.36) and p is the order of the generating LMM $[\rho(r), \sigma(r)]$ and SDLMM $[\rho(r), \sigma(r), \lambda(r)]$. Thus (2.39) therefore suggest that the difference $\alpha^{[j]} - \alpha$ in angle $\alpha^{[j]}$ of stability of $[\rho^{[j]}, \sigma^{[j]}]$ and α for $[\rho, \sigma]$ when the order of $[\rho, \sigma]$ is $p > 2$ deteriorates very rapidly. In fact, in the general case the difference deteriorates for an order of $p = 2$ of the k -step LMM $[\rho, \sigma]$ as $j \rightarrow \infty$. This conclusion is the same for (2.40).

Despite this discovered limitation of recursively applying (2.36),(2.14) and (2.15) as posited in theorem (2.12), arbitrarily high order $A(\alpha)$ -stable SDLMM (2.2) and LMM $[\rho(r), \sigma(r)]$ can readily be obtained by a careful choice of the parameter ε and a suitable generating method $[\rho(r), \sigma(r)]$ and $[\rho(r), \sigma(r), \lambda(r)]$ of order p small enough with limited recursivity of (2.36), (2.14) or (2.15) accordingly.

Methods arising from a recursive application of the process as in (2.14) and (2.15) shall be referred to as recursive SDBDF (RSDBDF). The stability region of once application of (2.14) and (2.15) for varying step number k of the SDBDF (2.19) are in Figs. 2b, 3a. The stability region of the weighted linear combination of the RSDBDF from (2.14) and (2.15) as defined in (2.27) for a corresponding k have been plotted as well in the Fig.3b. Take note that beyond the stated steplength k in the various graphs the resultant methods are unstable. Infact, the RSDBDF from (2.15) is unstable at $k = 6, 7, 8$, see Fig.3a for the stable region of $k = 1, 2, \dots, 5$.

3. THE IMEX SECOND DERIVATIVE LINEAR MULTISTEP METHODS

Consider a family of IMEX SDLMM to compute the numerical solution to the equation (1.2) of Prothero-Robinson type in (1.3). The section gives the derivation of *IMEX* methods up to order eight, following the approach in [1, 7, 9, 25]. The IMEX derived in this section are based on three categories which are, SDBDF (2.19), recursive formula in (2.20) and the weighted linear combination (2.27). The *IMEX* output of (2.20) will be employed for error control that of *IMEX* from (2.19).

(A*) The *IMEX* SDLMM approach can be generated as follows. Consider the implicit k -step method of SDBDF (2.19) of order $p = k + 1$ on (1.2), then

$$y_{n+k} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} = h\beta_k \left(f_{n+k} + g_{n+k} \right) + h^2 \lambda_k \left(f'_{n+k} + g'_{n+k} \right) \tag{3.1}$$

with f_{n+k}, f'_{n+k} - terms represented in an explicit form by applying the extrapolation,

$$\varphi(x_{n+k}) = \sum_{j=0}^{k-1} \gamma_j \varphi(x_{n+j}) + O(x^{q+1}); \varphi'(x_{n+k}) = \sum_{j=0}^{k-1} \gamma_j \varphi'(x_{n+j}) + O(x^{q+1}) \tag{3.2}$$

where $\varphi(x) = f(x, y(x))$ and $\varphi'(x) = f'(x, y(x))$. Then we have the *IMEX* SDLMM,

$$y_{n+k} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} = h \left(\sum_{j=0}^{k-1} \beta_j^* f_{n+j} + \beta_k g_{n+k} \right) + h^2 \left(\sum_{j=0}^{k-1} \lambda_j^* f'_{n+j} + \lambda_k g'_{n+k} \right) \tag{3.3}$$

$$\beta_j^* = \beta_j + \beta_k \gamma_j; \quad \lambda_j^* = \lambda_j + \lambda_k \gamma_j$$

The order of this IMEX is given by $\min(k + 1, q)$ with q being the order of the extrapolation in (3.2).

(B*) Following the approach in (A*) on (2.19), the IMEX SDLMM from the recursive

process (2.14) on a $(k - 1)$ -step SDBDF (2.19) of order $p = k$ is given as

$$\begin{aligned}
 y_{n+k}^* + \sum_{j=0}^{k-1} \alpha_j y_{n+j} &= h \left(\sum_{j=0}^{k-1} \beta_{j*}^* f_{n+j} + \beta_j g_{n+j} \right) + h \beta_k g_{n+k}^* \\
 &+ h^2 \left(\sum_{j=0}^{k-1} \lambda_{j*}^* f_{n+j} + \lambda_j g_{n+j} \right) + h^2 \lambda_k g_{n+k}^*; \\
 \beta_{j*}^* &= \beta_j + \beta_k \gamma_j; \quad \lambda_{j*}^* = \lambda_j + \lambda_k \gamma_j, \quad k \geq 2.
 \end{aligned}
 \tag{3.4}$$

This IMEX SDLMM shall be used for the error control through variation in the stepsize.

(C*) Similarly, the IMEX SDLMM based on a weighted linear combination of (2.14) and (2.15) in (2.27) is given as

$$\begin{aligned}
 y_{n+k}^{**} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} &= h \left(\sum_{j=0}^{k-1} \beta_{j*}^{**} f_{n+j} + \beta_j g_{n+j} \right) + h \beta_k g_{n+k}^{**} \\
 &+ h^2 \left(\sum_{j=0}^{k-1} \lambda_{j*}^{**} f'_{n+j} + \lambda_j g'_{n+j} \right) + h^2 \lambda_k g_{n+k}^{**}; \\
 \beta_{j*}^{**} &= \beta_j + \beta_k \gamma_j; \quad \lambda_{j*}^{**} = \lambda_j + \lambda_k \gamma_j, \quad k \geq 2.
 \end{aligned}
 \tag{3.5}$$

Theorem 3.1. *Let the implicit second derivative linear multistep method (2.2) or (2.19) be of order p and such that the extrapolation procedure (3.2) has order q then the IMEX method (3.2) has order $r = \min(p, q)$. In particular, if the IMEX SDLMM is based on the SDBDF (2.19) then $r = \min(k + 1, q)$.*

Proof. : With $\varphi(x) = f(x, y(x))$ and $\varphi'(x) = f'(x, y(x))$, the local truncation error (LTE) of the IMEX method (3.3) can be written as

$$\begin{aligned}
 LTE &= \frac{1}{h^2} \sum_{j=0}^k \left(\alpha_j y(x_{n+j}) - h \beta_j y'(x_{n+j}) - h^2 \lambda_j y'(x_{n+j}) \right) \\
 &+ \frac{1}{h} \beta_k \left(\varphi(x_{n+k}) - \sum_{j=0}^{k-1} \gamma_j \varphi(x_{n+j}) \right) + \lambda_k \left(\varphi'(x_{n+k}) \right. \\
 &\quad \left. - \sum_{j=0}^{k-1} \gamma_j \varphi'(x_{n+j}) \right) = Ch^{(p)} y^{(p)}(x_n) + O(h^{p+1}) \\
 &+ (\beta_k + \lambda_k) C' h^{(q)} \varphi^{(q)}(x_n) + O(h^{(q+1)}), \quad \alpha_k = 1
 \end{aligned}$$

The C and C' are the constants from the implicit method (2.2) and the extrapolation process (3.2) respectively. □

It follows that if the IMEX is based on the SDBDF (2.19) then $p = k + 1$ and $r = \min(k + 1, q)$.

3.1. Stability of the composite *IMEX* SDLMM in (3.3) - (3.5). Consider the stability properties of the *IMEX* SDLMM based on the SDBDF (2.19) which have been obtained from algorithms (3.1) to (3.4) for $k = 1, 2, \dots, 9$ respectively. The stability plots to be provided herein demonstrates that, some of the methods are unconditionally stable with respect to the step size h as their boundary loci plots will show in Figs. 6a,7a and 8a. This gives them an advantage over the linear multistep explicit methods which have severe restriction on the selection of stepsize for reason of stability requirement when solving stiff problems. In order to understand the stability behaviour of the schemes derived, we shall adopt the recent approach of Jorgenson [48] by using the test problem,

$$y'(x) = (e + \nu)\lambda y(x) - e\lambda y(x); \quad \text{Re}(\lambda) < 0, \quad 0 < e < \nu \quad (3.6)$$

This readily reduces to the Dahlquist test problem $y'(x) = \nu\lambda y(x)$. This $(e + \nu)\lambda y(x)$ is considered to be the stiff part $g(x, y(x))$ and $e\lambda y(x)$ is the non-stiff part $f(x, y(x))$ and the derivative of (3.6) is

$$y''(x) = (e + \nu)\lambda y'(x) - e\lambda y'(x)$$

This equation becomes

$$y''(x) = \lambda^2((e + \nu)^2 - 2e(e + \nu))y(x) + (e\lambda)^2 y(x)$$

Here the stiff part $g'(x, y(x))$ is $\lambda^2((e + \nu)^2 - 2e(e + \nu))y(x)$ and non-stiff $f'(x, y(x))$ part is $(e\lambda)^2 y(x)$. To fix ideas, consider the fourth order *IMEX* SDLMM.

Fourth-order *IMEX* SDLMM

The *IMEX* methods for $k = 4$ is given as

$$\begin{aligned} y_{n+4} - \frac{576}{415}y_{n+3} + \frac{216}{415}y_{n+2} - \frac{64}{85}y_{n+1} + \frac{9}{415}y_n = \frac{60}{83}h(-f_n \\ + 4f_{n+1} - 6f_{n+2} + 4f_{n+3} + g_{n+4}) - \frac{72}{415}h^2(-f'_n + 4f'_{n+1} \\ - 6f'_{n+2} + 4f'_{n+3} + g'_{n+4}); \end{aligned} \quad (3.7)$$

$$LTE = \frac{60}{83}y^{(5)}(x)h^5 + O(h^6) + \frac{24}{2075}y^{(6)}(x)h^6 + O(h^7), \quad p = 4$$

By applying on the scalar test problem (3.6), the following is obtained,

$$\begin{aligned} y_{n+4} - \frac{576}{415}y_{n+3} + \frac{216}{415}y_{n+2} - \frac{64}{85}y_{n+1} + \frac{9}{415}y_n = \frac{60}{83}h \left((-e\lambda)(-y_n \right. \\ \left. + 4y_{n+1} - 6y_{n+2} + 4y_{n+3}) + (e + \nu)y_{n+4} \right) - \frac{72}{415}h^2 \left((e\lambda)^2(-y_n \right. \\ \left. + 4y_{n+1} - 6y_{n+2} + 4y_{n+3}) + \left((e + \nu)^2 - 2e(e + \nu) \right) y_{n+4} \right) \end{aligned}$$

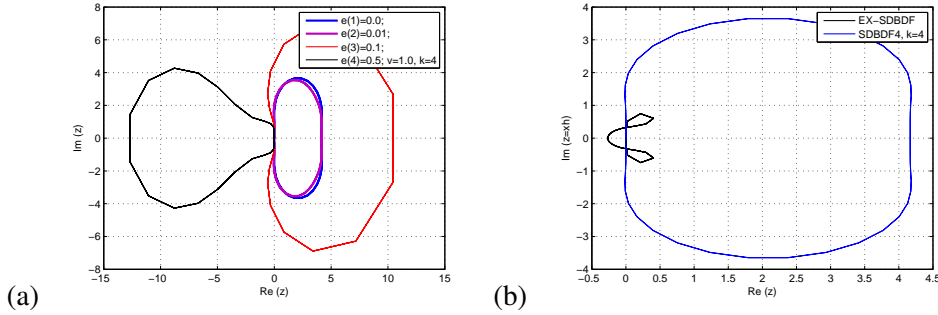


FIGURE 6. (a)-Stability plot of IMEX SDLMM (3.7) and (b)–SDBDF (2.19), $k = 4$ along with the explicit SDBDF, $k = 4$ seen around the origin

Replacing $h\lambda$ by $\frac{z}{\nu}$ results in

$$\begin{aligned}
 y_{n+4} - \frac{576}{415}y_{n+3} + \frac{216}{415}y_{n+2} - \frac{64}{85}y_{n+1} + \frac{9}{415}y_n &= \frac{60}{83}z \left(\frac{-e}{\nu}(-y_n \right. \\
 + 4y_{n+1} - 6y_{n+2} + 4y_{n+3}) + \frac{(e + \nu)}{\nu}y_{n+4} \Big) - \frac{72}{415}z^2 \left(\left(\frac{e}{\nu} \right)^2 (-y_n \right. \\
 + 4y_{n+1} - 6y_{n+2} + 4y_{n+3}) + \left. \left(\left(\frac{e + \nu}{\nu} \right)^2 - 2e \left(\frac{e + \nu}{\nu^2} \right) \right) y_{n+4} \right)
 \end{aligned}$$

Simplifying this,

$$\begin{aligned}
 &\left(1 - z \left(\frac{60(e + \nu)}{83\nu} \right) + \frac{72}{415}z^2 \left(\left(\frac{e + \nu}{\nu^2} \right)^2 - 2e \left(\frac{e + \nu}{\nu^2} \right) \right) \right) y_{n+4} \\
 &- \left(\frac{576}{415} - z \left(\frac{240e}{83\nu} \right) - \frac{288}{415}z^2 \left(\frac{e}{\nu} \right)^2 \right) y_{n+3} + \left(\frac{216}{415} - z \left(\frac{360e}{83\nu} \right) \right. \\
 &- \left. \frac{432}{415}z^2 \left(\frac{e}{\nu} \right)^2 \right) y_{n+2} - \left(\frac{64}{85} - z \left(\frac{240e}{83\nu} \right) - \frac{288}{415}z^2 \left(\frac{e}{\nu} \right)^2 \right) y_{n+1} \\
 &+ \left(\frac{9}{415} - z \left(\frac{60e}{83\nu} \right) - \frac{72}{415}z^2 \left(\frac{e}{\nu} \right)^2 \right) y_n = 0
 \end{aligned}$$

By setting $y_{n+j} \mapsto r^j$, $r = \exp^{i\theta}$, $0 \leq \theta \leq 2\pi$, the stability of the method in(3.7) can be studied for varying values of e and ν , through a boundary locus plot in Figs. 6a, 7 and 8a. The stability region is the exterior of the closed curves. The Fig. 6b is the plot for the independent explicit and implicit SDBDF (2.19) for $k = 4$ while the stability plot of the IMEX method (3.7) is given in Figs. 6a.

The Fig. 6a illustrates that the stability region of *IMEX* SDLMM is growing with e ; that is, the region of absolute stability grows as the scaling of the explicit part of the method approaches that of the implicit method. The method is *A*-stable when $\nu = 1.0$ with $e = 0.0, 0.01, 0.1$ and

at $e = 0.5$, it become method with limited stability region. The stability plots of the *IMEX* second derivative (3.3) for $k = 1, 2, 3, 5, 6, 7, 8, 9$ are in Figs. 7a and 8a.

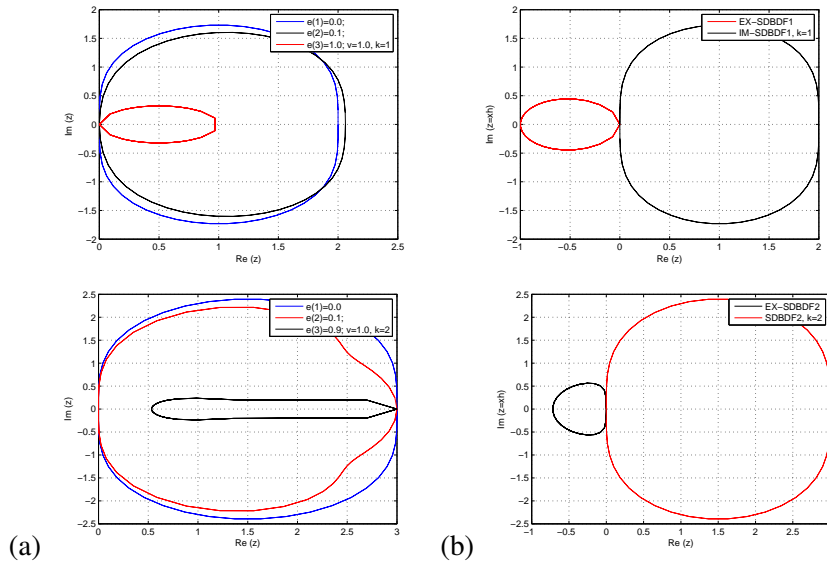


FIGURE 7. (a)– Stability plot of IMEX SDLMM (3.3) and (b)– SDBDF (2.19), $k = 1, 2$ along with the explicit SDBDF seen around the origin

4. STEPSIZE CONTROL OF THE IMEX SDLMM

The computational results from IMEX method can be significantly improved by varying the step size in the solution progress (3.3). The approach is to develop an estimate of the local truncation error which increase or decrease the stepsize appropriately in order to maintain a desire level for the error in the solution of (1.3), another way to have a better solution is to determine that the local error is smaller than a given tolerance. we take the advantage of this estimate to choose the better stepsize that will result in an acceptable error. We discuss adjustment of the stepsize in terms of local error by adapting the idea in [43, 49] to IMEX SDLMM (3.3). Given the stepsize of method (3.3) of order p is chosen in accordance to the PI-stepsize strategy

$$\begin{cases} y_{n+k} = (\text{as given by (3.3)}) \\ est(y_{n+k}) = y_{n+k} - y_{n+k}^* \\ h_{n+1} = h_n \left(\frac{\theta Tol}{||est(y_{n+k})||} \right)^{\frac{1}{(p+1)}}, \end{cases} \quad (4.1)$$

where θ is a control parameter chosen in a manner to reduce the number of rejected steps, Tol is a given error tolerance, and $est(y_{n+k})$ is an estimate of local discretization error in y_{n+k} which is taken as the difference between the IMEX SDLMM (3.3) and IMEX RSDLMM (3.4)

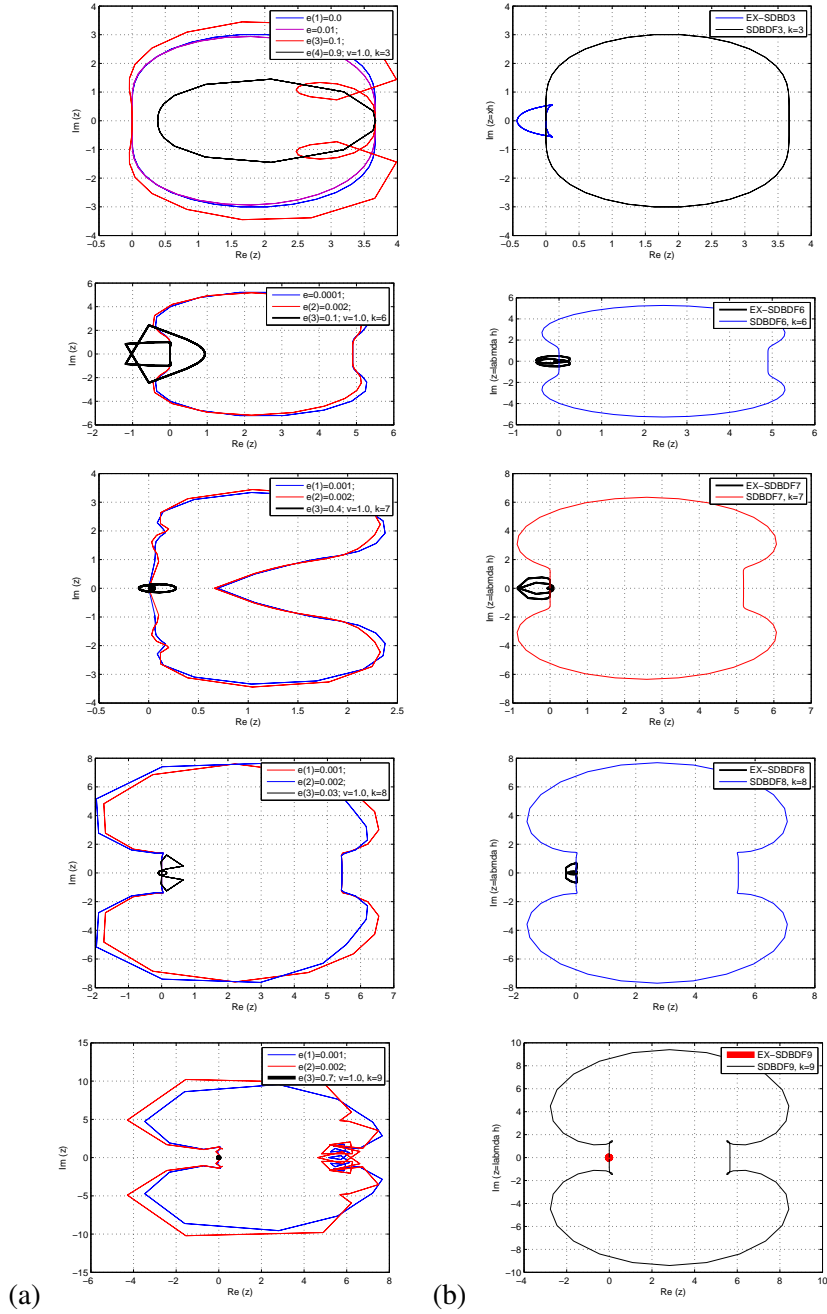


FIGURE 8. (a)– Stability plot of IMEX SDLMM (3.3) and (b)– SDBDF (2.19), $k = 3, 5, \dots, 9$ along with the explicit SDBDF seen around the origin

at x_{n+k} . An alternative to (4.1) is the PI-stepsize control given as

$$\begin{cases} y_{n+k} = (\text{as given by (3.3)}) \\ \text{est}(y_{n+k}) = y_{n+k} - y_{n+k}^* \\ h_{n+1} = h_n \left(\frac{\theta Tol}{|\text{est}(y_{n+k})|} \right)^\alpha \left(\frac{|\text{est}(y_{n+k-1})|}{\theta Tol} \right)^\beta, \end{cases}$$

with $\text{est}(y_{n+k-1})$ as an estimate of local discretization error at x_{n+k-1} which is taken as the difference between the solution of (3.3) and (3.5). The $\alpha = 0.175$ and $\beta = 0.089$ are constants. However, the alternative error estimate $\text{est}(y_{n+k}) = y_{n+k} - y_{n+k}^{**}$ in y_{n+k} from (3.4) can as well be adopted or even results of solution say y_{n+k} from (2.15) can be considered for error estimate too. We generalized algorithm in [49] to implement the IMEX SDLMM (3.3).

Algorithm: Step size selection in the IMEX SDLMM (3.3)

(1) **Given** Tolerance (Tol), initial condition $\{(x_0, y_0), (x_1, y_1), \dots, (x_{k-1}, y_{k-1})\}$
 Max_err, stepnumber of the IMEX SDLMM $k (\geq 1)$;

order of the method (p), constant $\alpha = 0.175, \beta = 0.089$

(2) Set the initial step size $h_0 = \frac{1}{10 \times 2^v}, v = 1 : 5, \theta = 0.9, n = 0$

(3) **Do**

{

(a) **Do**

{

(1) Compute y_{n+k} using (3.3)

(2) Compute $\text{est}(y_{n+k})$ i.e (the difference (3.3) – (3.4)) at x_{n+k}

(3) Compute $\text{est}(y_{n+k-1})$ i.e (the difference (3.3) – (3.5)) at x_{n+k-1}

if { $\text{est}(y_{n+k}) > \text{Max_err}$ **set** $\text{err1} = \text{Max_err}$ }

if { $|\text{est}(y_{n+k})| \leq Tol$

$\text{No_success_step} = \text{No_success_step} + 1$

$x_{n+k+1} = x_{n+k} + h_n, n=n+1$ (continue with next stepsize)}

if { $\text{err1} > Tol$ $\text{No_Fail_step} = \text{No_Fail_step} + 1$

(4) compute the new stepsize

$$h_{n+1} = \begin{cases} \theta * h_n \left(\frac{Tol}{\text{err1}} \right)^{\frac{1}{p+1}} \text{ or} \\ h_n \left(\frac{\theta Tol}{|\text{est}(y_{n+k})|} \right)^\alpha \left(\frac{|\text{est}(y_{n+k-1})|}{\theta Tol} \right)^\beta \end{cases}$$

}

Start the procedure with new stepsize h_{n+1}

}}

5. NUMERICAL IMPLEMENTATION ON SOME PROBLEMS

Consider some numerical experiments to illustrate the IMEX second derivative schemes (3.3) for solving (1.2). The implementation require the need to resolve the implicitness in the proposed IMEX second derivative schemes (3.3). The methods (3.3) for $k = 4, 5, 6, 7$ have been implemented to the Prothero-Robinson stiff problem in (1.3), while further implementation of the method (3.3) for $k = 5$ have been also considered on van der Pol equation and

Robertson’s equation. The implicitness in the IMEX methods (3.3) have been resolved using the Newton iterative scheme,

$$y_{n+k}^{(s+1)} = y_{n+k}^{(s)} - \left(J \left(y_{n+k}^{(s)} \right) \right)^{-1} F \left(y_{n+k}^{(s)} \right), \quad s = 0, 1, \dots, w. \quad (5.1)$$

for the IMEX method in (2.11) with $J \left(y_{n+k}^{(s)} \right) = \frac{\delta F \left(y_{n+k}^{(s)} \right)}{\delta y_{n+k}^{(s)}}$, as the Jacobian from (3.3), then

$$F \left(y_{n+k}^{(s)} \right) = y_{n+k}^{(s)} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} - h \left(\sum_{j=0}^{k-1} \beta_j^* f_{n+j} + \beta_k g \left(x_{n+k}, y_{n+k}^{(s)} \right) \right) - h^2 \left(\sum_{j=0}^{k-1} \lambda_j^* f'_{n+k} + \lambda_k g' \left(x_{n+k}, y_{n+k}^{(s)} \right) \right) = 0$$

in (5.1) and $J \left(y_{n+k} \right) = I - h \frac{\delta g \left(y_{n+k} \right)}{\delta y_{n+k}} - h^2 \frac{\delta g' \left(y_{n+k} \right)}{\delta y_{n+k}}$. The explicit SDBDF $y_{n+1} = y_n + h f_n + \frac{h^2}{2} f'_n$, $p = 2$, $C_3 = \frac{1}{6}$ for $k = 1$, has been used to generate the starting values for the Newton schemes in (5.1). The other methods in the family are implemented similarly.

Problem1: The stiff Prothero-Robinson test equation in [43],

$$\begin{cases} y'(x) = \lambda \left(y(x) - u(x) \right) + u'(x), & x \geq 0 \\ y(0) = u(0); \quad \lambda = -50, -100 \end{cases} \quad (5.2)$$

to be considered has the stiffness ratio $S = 50, 100$ respectively and the exact solution $y(x) = \left(y_0 - u(x_0) \right) \exp \left(\lambda \left(x - x_0 \right) + u(x) \right)$, where $u(x) = \sin \left(\frac{\pi}{4} + x \right)$.

Problem2: Van der Pol equations in ([42])

$$\begin{aligned} y_1' &= y_2 & y_2' &= -y_1 + 10y_2 \left(1 - y_1^2 \right) \\ y_1(0) &= 2, & y_2(0) &= 0 \end{aligned} \quad (5.3)$$

Table 6, contains the absolute error is given as the modulus of the ODE15s in MATLAB minus the numerical solution of the IMEX SDLMM.

Problem3: Robertson’s equation, see [42, 34] (nonlinear problem)

$$\begin{aligned} y_1' &= -0.004y_1 + 10^4 y_2 y_3, & y_2' &= 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2 \\ y_3' &= 3 \times 10^7 y_2^2, & y_1(0) &= 1, \quad y_2(0) = 0, \quad y_3 = 0 \end{aligned} \quad (5.4)$$

Table 7, contains the absolute error is given as the modulus of the ODE15s in MATLAB minus the numerical solution of the IMEX SDLMM.

Problem 4: the linear problem in [32]

$$y' = \begin{pmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \quad (5.5)$$

$$y(x) = \frac{1}{2} \begin{pmatrix} e^{-2x} + e^{-40x} (\cos(40x) + \sin(40x)) \\ e^{-2x} - e^{-40x} (\cos(40x) + \sin(40x)) \\ 2e^{-40x} (\cos(40x) - \sin(40x)) \end{pmatrix}.$$

The stiffness ratio of the problem (5.5) is $S = 28.5$. The problem in (5.5) is solved with a step length $h = \{0.05, 0.025, 0.0125, 0.00625\}$ within an interval $0 < x \leq 1$ using IMEX SDLMM of order $p = 6$. The maximum relative error $\max_{1 < i < 3} |y_i(x) - y_{i,h}| / (1 + |y_{i,h}|)$ viz the steplength is shown in Table 3. It was observed from the Table 3, that the IMEX SDLMM is favourably comparable with the SDBDF (2.19) of order $p = 6$. Here rate is the numerical order of convergence given in bracket and is given as

$$\begin{aligned} \text{rate} &= \log_2 \left(\frac{T_1}{T_2} \right); \quad i = 1(1)m, \quad m = 3, \quad 0 < x \leq 1 \\ T_1 &= \max_{1 < i < 3} |y_i(x) - y_{i,h}| / (1 + |y_{i,h}|) \\ T_2 &= \max_{1 < i < 3} |y_i(x) - y_{i,\frac{h}{2}}| / (1 + |y_{i,\frac{h}{2}}|) \end{aligned} \quad (5.6)$$

In Table 3, the rate is calculated from applying the IMEX SDLMM with two different step length h and $\frac{h}{2}$. Then, the rate is computed from the log of the absolute value of the ratio of two errors at the output point x . Where the exact solution is denoted by $y_i(x)$. In all, the rate is consistent with the order p of the respective methods in Table 3 with increasing steps or decreasing stepsize h .

TABLE 3. numerical results of problem 4 on interval $0 < x \leq 1$

h	IMEX SDLMM (y_{n+6}) (rate) $p = 6$	SDBDF6 (rate) $p = 6$
0.05	6.20×10^{-2} (-)	6.22×10^{-2} (-)
0.025	9.20×10^{-2} (2.75)	9.28×10^{-2} (2.74)
0.0125	5.61×10^{-4} (4.03)	5.72×10^{-4} (4.02)
0.00625	1.09×10^{-5} (5.68)	1.20×10^{-5} (5.57)

The maximum relative error from Ode15s at $t = 1$ is $3.660087954199254e - 5$ serving as a references solution.

The *IMEX* second derivative scheme based on SDBDF (2.19) for $k = 4, 5, 6, 7$ are;

$$\begin{aligned}
 y_{n+4} - \frac{576}{415}y_{n+3} + \frac{216}{415}y_{n+2} - \frac{64}{415}y_{n+1} + \frac{9}{415}y_n &= \frac{60}{83}h(-f_n \\
 + 4f_{n+1} - 6f_{n+2} + 4f_{n+3} + g_{n+4}) - \frac{72}{415}h^2 &(-f'_n + 4f'_{n+1} \\
 - 6f'_{n+2} + 4f'_{n+3} + g'_{n+4}), \quad k = 4, p = 4
 \end{aligned} \tag{5.7}$$

$$\begin{aligned}
 y_{n+5} + \frac{1}{12019}(-18000y_{n+4} + 9000y_{n+3} - 4000y_{n+2} + 1125y_{n+1} \\
 - 44y_n) = \frac{8220h}{12019}(5f_{n+4} - 10f_{n+3} + 10f_{n+2} - 5f_{n+1} + f_n + g_{n+5}) \\
 + \frac{1800}{12019}h^2(-f'_n + 5f'_{n+1} - 10f'_{n+2} + 10f'_{n+3} - 5f'_{n+4} - g'_{n+5}) \\
 k = 5, p = 5
 \end{aligned} \tag{5.8}$$

$$\begin{aligned}
 y_{n+6} + \frac{1}{13489}(-21600y_{n+5} + 13500y_{n+4} - 8000y_{n+3} + 3375y_{n+2} \\
 - 864y_{n+1} + 100y_n) = \frac{1220h}{1927}(6f_{n+5} - 15f_{n+4} + 20f_{n+3} - 15f_{n+2} \\
 + 6f_{n+1} - f_n - g_{n+6}) + \frac{1800}{13489}h^2(f'_n - 6f'_{n+1} + 15f'_{n+2} - 20f'_{n+3} \\
 + 15f'_{n+4} - 6f'_{n+5} - g'_{n+6}), k = 6, p = 6
 \end{aligned}$$

$$\begin{aligned}
 y_{n+7} + \frac{1}{726301}(-1234800y_{n+6} + 926100y_{n+5} - 686000y_{n+4} \\
 + 385875y_{n+3} - 148176y_{n+2} + 34300y_{n+1} - 3600y_n) \\
 = \frac{457380h}{726301}(7f_{n+6} - 21f_{n+5} + 35f_{n+4} - 35f_{n+3} + 21f_{n+2} - \\
 7f_{n+1} + f_n + g_{n+7}) + \frac{88200}{726301}h^2(-f'_n + 7f'_{n+1} - 21f'_{n+2} \\
 + 35f'_{n+3} - 35f'_{n+4} + 21f'_{n+5} - 7f'_{n+6} - g'_{n+7}), k = 7, p = 7
 \end{aligned}$$

The *IMEX* (3.4) at $k = 4$ used for error control is given as

$$\begin{aligned}
 y_{n+4} - \frac{301}{170}y_{n+3} + \frac{81}{85}y_{n+2} - \frac{7}{34}y_{n+1} + \frac{2}{85}y_n &= -h \left(\frac{1}{85} \left(-66f_n \right. \right. \\
 + 264f_{n+1} - 396f_{n+2} + 231f_{n+3} \Big) - \frac{9}{8500}g_n + \frac{9}{2125}g_{n+1} - \\
 \frac{27}{4250}g_{n+2} - \frac{48}{125}g_{n+3} + \frac{6591}{8500}g_{n+4} \Big) - h^2 \left(\frac{1}{8500} \left(-1881f'_n \right. \right. \\
 + 7443f'_{n+1} - 11043f'_{n+2} + 6381f'_{n+3} - 81g'_n \\
 \left. \left. + 243g'_{n+1} - 243g'_{n+2} - 819g'_{n+3} + 1800g'_{n+4} \right) \right)
 \end{aligned}$$

TABLE 4. Numerical solution to problem in (5.2) with $\lambda = -50$, $x=1.0$, $y(1)=9.77061e-001$

h	Methods (k)	Tol	$\frac{Acceptedstep}{Totalstep}$	Error in IMEX SDLMM	Error in SDBDF
10^{-2}	4			3.01645e-03	3.01615e-03
	5	10^{-3}	$\frac{14}{14}$	3.06876e-03	3.06851e-03
	6	10^{-3}	$\frac{22}{27}$	6.63855e-04	5.54453e-04
	7	10^{-3}	$\frac{15}{15}$	5.96364e-03	4.126011e-03
10^{-3}	4			4.145269e-03	4.14524e-03
	5			4.15324e-03	4.15322e-03
	6	10^{-3}	$\frac{45}{45}$	1.21580e-03	3.16496e-04
	7			4.24158e-03	4.21425e-03
10^{-4}	4			3.73762e-03	3.73761e-03
	5	10^{-3}	$\frac{140}{140}$	3.73835e-03	3.73834e-03
	6			1.52303e-03	7.35311e-04
	7			3.74562e-03	3.74321e-03

Error control IMEX methods for $k = 1, 2, 3, 5, 6, 7, 8, 9$ for method (3.4) can be obtained similarly using the extrapolation (3.2). Implementing on Prothero-Robinson test problem (5.2) based on the splitting in (3.6), the stiff term is $g = (\epsilon + \nu)\lambda y - \lambda u(x)$ and the non-stiff term is $f = -\epsilon\lambda y + u'(x)$ with $e = 0.001$ and $\nu = 1.0$ in the stable schemes (3.3).

The *IMEX* SDLMM methods (3.3) resolves the implicitness in the numerical solution of (1.2) in a cost effective way. The problems have been solved using the *IMEX* SDLMM (5.3)-(5.8) and also by the SDBDF (2.19) for $k = 4$ (1) 7 and they have produced the same numerical order of accuracy as seen in the tables 1, 2. We observe the number of step increases like $O(n^2)$ depend on the chosen tolerance.

In Figs. 9 and 10, we see that numerical solutions from the method (3.3) for $k = 5$ in problem 2 and 3 respectively coincide with the solution from ODE15s. From Table 6 and 7. This confirms that the method in (3.3) performs as well as the conventional SDBDF for $k = 5$.

6. CONCLUSION

The recursive derivation of high order $A(\alpha)$ -stable SDLMM (2.14) and (2.15) have been introduced in this work in section 2 along with new further theoretic insight into general SDLMM in (2.1). The *IMEX* methods derived in section 3 are A -stable for $k = 1, 2, 3$ and $A(\alpha)$ -stable for $k = 4, 5, 6, 7$. The proposed *IMEX* second derivative method (3.3) has been implemented

TABLE 5. Numerical solution to problem in (5.2) with $\lambda = -100$, $x=1.0$, $y(1)=9.77061e-001$

h	Methods (k)	Tol	$\frac{Acceptedstep}{Totalstep}$	Error in IMEX SDLMM	Error in SDBDF
10^{-2}	4	10^{-3}	$\frac{14}{14}$	1.78664e-03	1.78608e-03
	5			1.84603e-03	1.84555e-03
	6			3.72596e-03	6.95988e-03
	7			6.36788e-03	4.38210e-03
10^{-3}	4	10^{-3}	$\frac{45}{45}$	2.10997e-03	2.10995e-03
	5			2.11766e-03	2.11764e-03
	6			8.81910e-04	1.56477e-04
	7			2.25285e-03	2.19058e-03
10^{-4}	4	10^{-3}	$\frac{140}{140}$	1.87222e-03	1.87222e-03
	5			1.87292e-03	1.87292e-03
	6			1.14456e-03	3.44261e-04
	7			1.88298e-03	1.87807e-03

TABLE 6. Numerical results in comparison with SDBDF5 for problem 2, $h = 10^{-3}$

x	y_i	Error in IMEX SDLMM	Error in SDBDF5
1.0	y_1	2.7969345e-04	2.7968394e-04
	y_2	1.3151054e-03	1.3148005e-03
10.0	y_1	5.3686752e-04	5.3685832e-04
	y_2	1.3226643e-03	1.3223581e-03
20.0	y_1	1.4210197e-04	1.3212439e-04
	y_2	1.3226643e-03	1.3215489e-03
40.0	y_1	1.6256519e-03	1.6256418e-03
	y_2	1.172168e-03	1.1718652e-03

The Error in IMEX SDLMM= $|y_i(3.3) - y_i(Ode15s)|$ and Error in SDBDF5= $|y_i(2.19) - y_i(Ode15s)|, i = 1, 2.$

on some well-known stiff initial value problem with results in Tables 4, 5, 6, 7 showing reasonable accuracy when compared to the exact solution (5.2) and Ode15s as Figs. 9 and 10 show. The LTE is the difference between the proposed IMEX SDLMM (3.3) and IMEX SDLMM

TABLE 7. Numerical results in comparison with SDBDF5 for problem 3, $h = 10^{-4}$

x	y_i	Error in IMEX SDLMM (y_{n+5})	Error in SDBDF5
1.0	y_1	1.4618195e-05	1.4618001e-05
	y_2	2.3356540e-09	2.3356219e-09
	y_3	1.4620462e-05	1.4620268e-05
10.0	y_1	7.5877914e-05	7.5877860e-05
	y_2	5.9556380e-09	5.9556329e-09
	y_3	7.5883862e-05	7.5883808e-05
20.0	y_1	1.1381697e-04	1.1381694e-04
	y_2	6.3702360e-09	6.3702340e-09
	y_3	1.1382334e-04	1.1382330e-04
40.0	y_1	1.0530473e-04	1.0530461e-04
	y_2	4.0599400e-09	4.0599090e-09
	y_3	1.0530879e-04	1.0530877e-04

The Error in IMEX SDLMM= $|y_i(3.3) - y_i(Ode15s)|$ and Error in SDBDF5= $|y_i(2.19) - y_i(Ode15s)|, i = 1, 2, 3.$

(3.4) from recursive SDLMM. The scheme proposed herein are suitable for the numerical solution of ordinary differential equations from spatial discretization of partial differential equations using the method of lines and also from other application for which the arising ordinary differential equations is amenable to the additive splitting in (1.2).

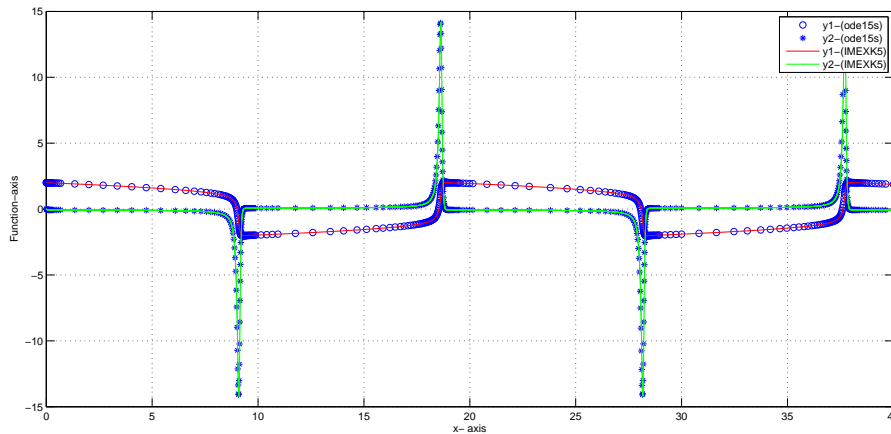


FIGURE 9. Numerical results for problem 2 using IMEX SDLMM (3.3) for k=5

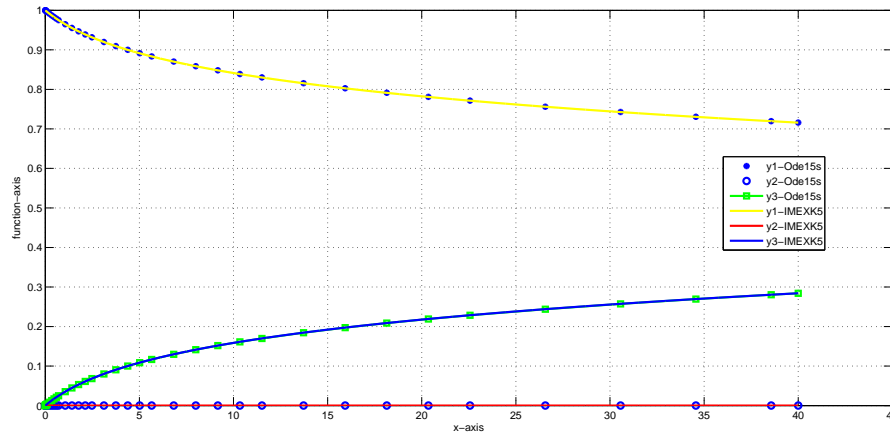


FIGURE 10. Numerical results for problem 3 using IMEX SDLMM (3.3) for $k=5$

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