Applied Numerical Mathematics 183 (2023) 15–38

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

3-additive linear multi-step methods for diffusion-reaction-advection models

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A R T I C L E   I N F O

Article history:
Received 23 August 2021
Received in revised form 27 July 2022
Accepted 18 August 2022
Available online 27 August 2022

Keywords:
Additive splitting methods
Linear multi-step methods
Diffusion-reaction-advection problems
IMEX
Order conditions
Linear stability analysis

A B S T R A C T

Some systems of differential equations that model problems in science and engineering have natural splittings of the right-hand side into the sum of three parts, in particular, diffusion, reaction, and advection. Implicit-explicit (IMEX) methods treat these three terms with only two numerical methods, and this may not be desirable. Accordingly, this work gives a detailed study of 3-additive linear multi-step methods for the solution of diffusion-reaction-advection systems. Specifically, we construct new 3-additive linear multi-step methods that treat diffusion, reaction, and advection with separate methods. The stability of the new methods is investigated, and the order of convergence is tested numerically. A comparison of the new methods is made with some popular IMEX methods in terms of stability and performance. It is found that the new 3-additive methods have larger stability regions than the IMEX methods tested in some cases and generally outperform in terms of computational efficiency.

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1. Introduction

Many important systems modeled by partial differential equations (PDEs) have natural additive splittings according to physical contributions, e.g., diffusion-reaction-advection (DRA) PDEs. DRA PDEs describe the movement of substances from an area of high concentration to an area of low concentration (diffusion), the chemical transformation of a set of substances into others (reaction), and the movement of substances from one region to another (advection). For instance, DRA PDEs are used to model air pollution [30,40], combustion [9], the Heston model of financial mathematics [23], tumor angiogenesis and chemo-taxis [27], heat conduction [7,8,31], hemodynamics [18,36], blood coagulation [11,33], cardiac arrhythmias [15,35], and atherosclerosis [20,24].

Many DRA equations include nonlinear terms, and this leads to difficulties in obtaining analytic solutions. Therefore, approximating the solution via numerical methods is often the only feasible option. In general, popular numerical methods for solving ordinary differential equations (ODEs) are applied to the large systems of ODEs that result from the spatial discretization of DRA PDEs by, e.g., finite difference methods, finite element methods, finite volume methods, or pseudospectral methods [27].

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https://doi.org/10.1016/j.apnum.2022.08.015
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A popular and effective approach to obtain a numerical solution to DRA PDEs is through the application of an implicit-explicit (IMEX) method. In a typical version of this approach, the diffusion and reaction terms are treated implicitly in time, and the advection terms are treated explicitly. The idea of IMEX splitting, which was proposed as a partitioned method, dates back to the late 1970s in [19,25]. It was proposed as a multi-step method in 1980 [16]. After that, many other classes of IMEX methods were studied. For instance, IMEX linear multi-step methods (LMMs) were derived in [6,34] and were investigated in many studies, e.g., [5,17,26,27,34,37]. The stability properties of IMEX methods are often studied on the basis of stability regions defined by using complex scalar test equations; see [2–4,6,21,34]. Higher-order methods and those with other enhanced numerical properties such accuracy, error analysis, monotonicity, and boundedness were studied in [27,28,32]. Classes of general linear IMEX methods were developed in [12,13,38,39].

IMEX methods are a class of 2-additive methods. When dealing with DRA PDEs, this constraint necessitates a grouping of three physical processes into two and could be undesirable depending on the specific problem. For example, if the reaction term is nonlinear and stiff, then treating diffusion and reaction implicitly together may be much less desirable than treating them separately. In the latter case, the diffusion is often linear, and reaction term usually leads to a system of uncoupled ODEs; i.e., both of these sub-problems have specialized solvers associated with them that cannot be taken advantage of when combined. Furthermore, the relative importance of the terms may change during a simulation, again making the choice of an IMEX method sub-optimal. In this work, we investigate two classes of linear multi-step methods that treat diffusion, reaction, and advection separately, i.e., 3-additive methods.

Consider the initial-value problem (IVP) for a system of ODEs of the form

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t}(t) = \mathbf{f}^{[1]}(t,\mathbf{y}) + \mathbf{f}^{[2]}(t,\mathbf{y}) + \mathbf{f}^{[3]}(t,\mathbf{y}), \quad t \in [t_0, T], \tag{1a}$$

$$\mathbf{y}(t_0) = \mathbf{y}_0, \tag{1b}$$

where it is assumed that IVP (1) comes from a spatial discretization of an DRA problem and the functions $\mathbf{f}^{[i]} : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$, $i = 1, 2$, and 3, and dimension $m \geq 1$, are assumed to be sufficiently smooth.

A 3-additive numerical solution of equation (1) can be found by writing the exact integration of the right-hand side from t_n to t_{n+1}:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \int_{t_n}^{t_{n+1}} \left(\mathbf{f}^{[1]}(t,\mathbf{y}(t)) + \mathbf{f}^{[2]}(t,\mathbf{y}(t)) + \mathbf{f}^{[3]}(t,\mathbf{y}(t))\right) dt$$

and then using quadrature to approximate the integrals of $\mathbf{f}^{[1]}$, $\mathbf{f}^{[2]}$, and $\mathbf{f}^{[3]}$ by different methods. For example, if the integral of the first term is approximated by backward Euler method, the integral of the second term is approximated by trapezoidal method, and the integral of the last term is approximated by forward Euler method, one can obtain the following formula:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t\, \mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1}) + \frac{\Delta t}{2}\left(\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1}) + \mathbf{f}^{[2]}(t_n,\mathbf{y}_n)\right) + \Delta t\, \mathbf{f}^{[3]}(t_n,\mathbf{y}_n). \tag{2}$$

The formula (2) is an example of 3-additive numerical method.

The functions $\mathbf{f}^{[1]}$, $\mathbf{f}^{[2]}$, and $\mathbf{f}^{[3]}$ correspond to the spatial discretizations of the diffusion, reaction, and advection terms, respectively. The function $\mathbf{f}^{[1]}$ is assumed to be a stiff term that is to be integrated implicitly, whereas $\mathbf{f}^{[3]}$ is assumed to be a nonstiff term that is to be integrated explicitly. The function $\mathbf{f}^{[2]}$ could be stiff or non-stiff and hence could be treated either implicitly or explicitly, yielding Implicit-Implicit-Explicit (IIE) or Implicit-Explicit-Explicit (IEE) methods, respectively.

The remainder of the paper is organized as follows. The class of k-step IIE linear multi-step methods is described in section 2. The stability of IIE methods is investigated for a linear DRA PDE in section 2.1. Some IIE methods up to fourth order are derived in section 3. The class of k-step IEE linear multi-step methods is described in section 4. The linear stability of IEE methods is investigated for a linear DRA in section 4.1. Some IEE methods up to third order are derived in section 5. Some numerical experiments that verify the convergence order and illustrate the performance of 3-additive splitting methods compared to popular IMEX methods are presented in section 6. The results are generalized to N-additive methods in section 7. Conclusions are given in section 8.

We compare IIE-LMMs and IEE-LMMs with IMEX methods, respectively, in terms of stability and performance. Using the following approaches in the comparison between IIE-LMMs and IMEX methods, when applying IMEX methods to the ODE of the form

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} = \mathbf{g}(t,\mathbf{y}) + \mathbf{f}(t,\mathbf{y}). \tag{3}$$

In the comparison between IIE-LMMs and IMEX methods, the diffusion and reaction terms are treated implicitly, and their discretizations are grouped together as part of $\mathbf{g}(t,\mathbf{y})$; the advection term is treated explicitly, and its discretization corresponds to $\mathbf{f}(t,\mathbf{y})$. In other words, $\mathbf{g}(t,\mathbf{y}) = \mathbf{f}^{[1]}(t,\mathbf{y}) + \mathbf{f}^{[2]}(t,\mathbf{y})$ and $\mathbf{f}(t,\mathbf{y}) = \mathbf{f}^{[3]}(t,\mathbf{y})$. In the comparison between IEE-LMMs and IMEX methods, the diffusion term is treated implicitly, and its discretization corresponds to $\mathbf{g}(t,\mathbf{y})$; the advection and reaction terms are treated explicitly, and their discretizations are grouped together as part of $\mathbf{f}(t,\mathbf{y})$. In other words, $\mathbf{g}(t,\mathbf{y}) = \mathbf{f}^{[1]}(t,\mathbf{y})$ and $\mathbf{f}(t,\mathbf{y}) = \mathbf{f}^{[2]}(t,\mathbf{y}) + \mathbf{f}^{[3]}(t,\mathbf{y})$.

2. k-step IIE linear multi-step methods

We now derive k-step IIE methods for (1), $k \geq 1$. Let $\mathbf{y}_n$ represent the approximate solution at $t_n = t_0 + n\Delta t$, where Δt is the discretization step size. Then, the IIE linear multi-step method with k steps can be defined by

$$\frac{1}{\Delta t}\mathbf{y}_{n+1} + \frac{1}{\Delta t}\sum_{j=0}^{k-1} a_j \mathbf{y}_{n-j} = \sum_{j=-1}^{k-1} b_j^{[1]}\mathbf{f}^{[1]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=-1}^{k-1} b_j^{[2]}\mathbf{f}^{[2]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=0}^{k-1} b_j^{[3]}\mathbf{f}^{[3]}(t_{n-j},\mathbf{y}_{n-j}), \tag{4}$$

where we assume that $b_{-1}^{[1]}, b_{-1}^{[2]} \neq 0$. Expanding (4) in Taylor series about t_n to obtain the truncation error yields

$$\begin{aligned}
&\frac{1}{\Delta t}\left[1+\sum_{j=0}^{k-1} a_j\right]\mathbf{y}(t_n) + \left[1-\sum_{j=1}^{k-1} j a_j\right]\mathbf{y}^{(1)}(t_n) + \cdots + \frac{(\Delta t)^{p-1}}{(p)!}\left[1+\sum_{j=1}^{k-1}(-j)^p a_j\right]\mathbf{y}^{(p)}(t_n) = \\
&\sum_{j=-1}^{k-1} b_j^{[1]}\mathbf{f}^{[1]}(\mathbf{y}(t_n)) + \Delta t\left[b_{-1}^{[1]} - \sum_{j=1}^{k-1} j b_j^{[1]}\right]\frac{\mathrm{d}\mathbf{f}^{[1]}}{\mathrm{d}t}\Big|_{t=t_n} + \cdots + \frac{(\Delta t)^{p-1}}{(p-1)!}\left[b_{-1}^{[1]} + \sum_{j=1}^{k-1}(-j)^{p-1} b_j^{[1]}\right]\frac{\mathrm{d}^{p-1}\mathbf{f}^{[1]}}{\mathrm{d}t^{p-1}}\Big|_{t=t_n} + \\
&\sum_{j=-1}^{k-1} b_j^{[2]}\mathbf{f}^{[2]}(\mathbf{y}(t_n)) + \Delta t\left[b_{-1}^{[2]} - \sum_{j=1}^{k-1} j b_j^{[2]}\right]\frac{\mathrm{d}\mathbf{f}^{[2]}}{\mathrm{d}t}\Big|_{t=t_n} + \cdots + \frac{(\Delta t)^{p-1}}{(p-1)!}\left[b_{-1}^{[2]} + \sum_{j=1}^{k-1}(-j)^{p-1} b_j^{[2]}\right]\frac{\mathrm{d}^{p-1}\mathbf{f}^{[2]}}{\mathrm{d}t^{p-1}}\Big|_{t=t_n} + \\
&\sum_{j=0}^{k-1} b_j^{[3]}\mathbf{f}^{[3]}(\mathbf{y}(t_n)) - \Delta t\sum_{j=1}^{k-1} j b_j^{[3]}\frac{\mathrm{d}\mathbf{f}^{[3]}}{\mathrm{d}t}\Big|_{t=t_n} + \cdots + \frac{(\Delta t)^{p-1}}{(p-1)!}\sum_{j=1}^{k-1}(-j)^{p-1} b_j^{[3]}\frac{\mathrm{d}^{p-1}\mathbf{f}^{[3]}}{\mathrm{d}t^{p-1}}\Big|_{t=t_n} + \mathcal{O}((\Delta t)^p).
\end{aligned} \tag{5}$$

Using (1) in the truncation error (5) leads to the order conditions

$$\begin{aligned}
&1+\sum_{j=0}^{k-1} a_j = 0, \\
&1-\sum_{j=1}^{k-1} j a_j = \sum_{j=-1}^{k-1} b_j^{[1]} = \sum_{j=-1}^{k-1} b_j^{[2]} = \sum_{j=0}^{k-1} b_j^{[3]}, \\
&\frac{1}{2}+\sum_{j=1}^{k-1}\frac{j^2}{2} a_j = b_{-1}^{[1]} - \sum_{j=1}^{k-1} j b_j^{[1]} = b_{-1}^{[2]} - \sum_{j=1}^{k-1} j b_j^{[2]} = -\sum_{j=1}^{k-1} j b_j^{[3]}, \\
&\qquad\vdots \\
&\frac{1}{p!}+\sum_{j=1}^{k-1}\frac{(-j)^p}{p!} a_j = \frac{b_{-1}^{[1]}}{(p-1)!} + \sum_{j=1}^{k-1}\frac{(-j)^{p-1} b_j^{[1]}}{(p-1)!} = \frac{b_{-1}^{[2]}}{(p-1)!} + \sum_{j=1}^{k-1}\frac{(-j)^{p-1} b_j^{[2]}}{(p-1)!} = \sum_{j=1}^{k-1}\frac{(-j)^{p-1} b_j^{[3]}}{(p-1)!}.
\end{aligned} \tag{6}$$

The system (6) gives the conditions for a k-step IIE-LMM to have order p. The following theorem investigates the maximal order for a given k.

Theorem 1. *For the k-step IIE-LMM (4), we have:*

I. If $p \leq k$, then the $3p+1$ conditions of the system (6) are linearly independent. So there exist k-step IIE-LMMs of order k.
II. The order of accuracy of a k-step IIE-LMM is at most k.
III. The family of k-step IIE-LMMs of order k has $k+1$ free parameters.

Proof. I. Because linear independence for $p = k$ implies linear independence for $p \leq k$, it is sufficient to prove the case $p = k$ only. The system (6) can be represented in matrix form

$$\mathbf{WV} = \mathbf{U}, \tag{7}$$

where

$$\begin{aligned}
&\mathbf{V} = [a_0, \ldots, a_{k-1}, b_{-1}^{[1]}, b_0^{[1]}, \ldots, b_{k-1}^{[1]}, b_{-1}^{[2]}, b_0^{[2]}, \ldots, b_{k-1}^{[2]}, b_0^{[3]}, b_1^{[3]}, \ldots, b_{k-1}^{[3]}]^T \in \mathbb{R}^{4k+2}, \\
&\mathbf{U} = [-1, \ldots, -1_{k+1}, 0, \ldots, 0_{2k}]^T \in \mathbb{R}^{3k+1},
\end{aligned}$$

and

$$\mathbf{W} = \left[\begin{array}{c|c|cccc} \mathbf{A} & \mathbf{L} & 0 & \dots & \dots & 0 \\ \mathbf{H} & & -\mathbf{DA} & \mathbf{0} & \dots & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{1} & \mathbf{A} & -\mathbf{1} & -\mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{A} & -\mathbf{A} \end{array}\right]_{(3k+1)\times(4k+2)},$$

with

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 0 & -1 & -2 & \dots & 1-k \\ 0 & 1 & 4 & \dots & (1-k)^2 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & (-1)^{k-1} & (-2)^{k-1} & \dots & (1-k)^{k-1} \end{bmatrix}_{k\times k}, \tag{8}$$

$$\mathbf{D} = \begin{bmatrix} 1 & & & \\ & 2 & & \\ & & \ddots & \\ & & & k \end{bmatrix}_{k\times k}, \tag{9}$$

$$\mathbf{H} = \left[0, (-1)^k, \dots, (1-k)^k\right]_{1\times k}, \tag{10}$$

$$\mathbf{L} = \left[0, -1, -2, \dots, -k\right]^T_{1\times(k+1)}, \tag{11}$$

and $\mathbf{1}$ is a vector of ones with size k. The matrix $\mathbf{A}$ is a Vandermonde matrix for the distinct numbers $\{0, -1, -2, \dots, 1-k\}$. Because the Vandermonde matrix $\mathbf{A}$ is nonsingular [22], it can be noted that columns $1, k+2, \dots, 2k+1, 2k+3, \dots, 4k+2$, of the matrix $\mathbf{W}$ are linearly independent. Thus, all $(3p+1)$ conditions are linearly independent, and the system (6) admits a $(4k-3p+1)$-parameter family of solutions for $p \le k$. Because columns $(k+1)$ and $(2k+2)$ of matrix $\mathbf{W}$ do not enter into the above proof, we know $b^{[1]}_{-1}$ and $b^{[2]}_{-1}$ can have any nonzero value. This property verifies that the family of methods is IIE-LMM.

II. Assume the IIE-LMM has accuracy $\mathcal{O}((\Delta t)^{k+r})$, $r \ge 1$; then the following conditions should be satisfied:

$$\begin{aligned} \sum_{j=-1}^{k-1} b^{[2]}_j &= \sum_{j=0}^{k-1} b^{[3]}_j, \\ b^{[2]}_{-1} + \sum_{j=1}^{k-1}(-j)b^{[2]}_j &= \sum_{j=1}^{k-1}(-j)b^{[3]}_j, \\ &\vdots \\ b^{[2]}_{-1} + \sum_{j=1}^{k-1}(-j)^k b^{[2]}_j &= \sum_{j=1}^{k-1}(-j)^k b^{[3]}_j. \end{aligned} \tag{12}$$

Let $\mu_j = b^{[2]}_j - b^{[3]}_j$; then the system (12) can be written as

$$\begin{aligned} b^{[2]}_{-1} + \sum_{j=0}^{k-1}\mu_j &= 0, \\ b^{[2]}_{-1} + \sum_{j=1}^{k-1}(-j)\mu_j &= 0, \\ &\vdots \\ b^{[2]}_{-1} + \sum_{j=1}^{k-1}(-j)^k\mu_j &= 0. \end{aligned} \tag{13}$$

Writing the system (13) in a matrix form yields

$$\begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 0 & -1 & \dots & 1-k \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & 0 & (-1)^k & \dots & (1-k)^k \end{bmatrix}_{(k+1)\times(k+1)} \begin{bmatrix} b_{-1}^{[2]} \\ \mu_0 \\ \vdots \\ \mu_{k-1} \end{bmatrix}_{(k+1)\times 1} = \mathbf{0},$$

implying that $b_{-1}^{[2]} = 0$ and $b_j^{[2]} = b_j^{[3]}$, $j = 1, 2, \dots, k-1$, because the matrix of coefficients is nonsingular. This contradicts the assumption $b_{-1}^{[2]} \neq 0$.

III. Consider a k-step IIE-LMM that achieves the maximal order. Then, as shown above, the family of such method has exactly $(k+1)$ free parameters. □

2.1. Linear stability analysis for IIE-LMMs

Consider the scalar test problem

$$\frac{dy}{dt} = -\mu^2 y + \lambda y + i\nu y, \tag{14}$$

where $\mu, \nu \in \mathbb{R}$, $\lambda = \lambda_r + i\lambda_i \in \mathbb{C}$, and $\lambda_r, \lambda_i \in \mathbb{R}$. The terms in the test problem are meant to represent typical eigenvalues of the Jacobians of $\mathbf{f}^{[i]}$, $i = 1, 2, 3$, with respect to the solution $\mathbf{y}$, assuming they are simultaneously diagonalizable. Specifically, $-\mu^2 y$ corresponds to the diffusion term, λy corresponds to the reaction term, and $i\nu y$ corresponds to the advection term.

Applying IIE-LMM (4) to (14) yields

$$\left[1 + \Delta t b_{-1}^{[1]} \mu^2 - \Delta t b_{-1}^{[2]} (\lambda_r + i\lambda_i)\right] y_{n+1} + \sum_{j=0}^{k-1} \left[a_j - i\Delta t (b_j^{[2]} \lambda_i + b_j^{[3]} \nu) + \Delta t \mu^2 b_j^{[1]} - \Delta t b_j^{[2]} \lambda_r\right] y_{n-j} = 0.$$

Assuming this linear constant-coefficient difference equation has solutions of the form $y_n = \xi^n$, then the characteristic equation is given by

$$\Phi(\xi) \equiv \left[1 + \Delta t (b_{-1}^{[1]} \mu^2 - b_{-1}^{[2]} \lambda_r) - i\Delta t b_{-1}^{[2]} \lambda_i\right] \xi^k + \sum_{j=0}^{k-1} \left[a_j - i\Delta t (b_j^{[2]} \lambda_i + b_j^{[3]} \nu) + \Delta t (\mu^2 b_j^{[1]} - b_j^{[2]} \lambda_r)\right] \xi^{k-j-1}. \tag{15}$$

It can be noted that the stability holds if and only if all simple roots of the equation (15) satisfy $|\xi_j| \leq 1$ and multiple roots satisfy $|\xi_j| < 1$. The region in complex plane that contains these roots is called the stability region of the method. However, the stability region of 3-additive methods is in $\mathbb{C}^2$ ($\simeq \mathbb{R}^4$). It is not entirely obvious how to characterize the stability behavior of a 3-additive LMM by adjusting the parameters μ, ν, and λ. To overcome this difficulty, we discuss the stability of IIE-LMMs in three cases $\lambda = i\nu$, $\lambda = -\mu^2$ and $\lambda = -\mu^2 + i\nu$. These cases represent the limits of the reaction term having purely imaginary eigenvalues, purely negative real eigenvalues, and the intermediate case where it has an equal combination of the two.

3. Construction and stability of IIE-LMMs

In this section, we construct IIE-LMMs by using the coefficients of well-known IMEX methods for the $\mathbf{f}^{[1]}$ (diffusion) and $\mathbf{f}^{[2]}$ (reaction) terms, and then derive coefficients of $\mathbf{f}^{[3]}$ (advection) terms that satisfy the relevant order conditions (6). The order conditions for IIE-LMMs methods are summarized in Table A.5. We then also analyze the linear stability of the constructed methods using eq. (14) in the three cases described. The linear stability regions for IIE-LMMs up to fourth order are presented in Table 2.

First-order IIE methods

The two-parameter family of one-step, first-order IIE-LMMs for (1) is presented in Table 1. The choice $(\alpha, \beta) = (1, \frac{1}{2})$ in IIE1 yields the formula (2), which was used to introduce 3-additive splitting methods in section 1.

Stability analysis

Applying the method IIE1 to the test equation (14) yields the stability region $\{|\xi(\nu, \lambda, \mu)| \leq 1\}$, where

$$\begin{aligned} \xi(\nu, \lambda, \mu) &= 1 + \frac{i\Delta t\nu - \Delta t\mu^2 + \Delta t\lambda}{1 + \Delta t(\alpha\mu^2 - \beta\lambda)}, \\ &= 1 + \frac{\Delta t(\lambda_r - \mu^2) + i\Delta t(\nu + \lambda_i)}{1 + \Delta t(\alpha\mu^2 - \beta\lambda_r) - i\Delta t\beta\lambda_i}. \end{aligned} \tag{16}$$

Table 1
IIE-LMMs.

k	Methods	
$k=1$	$\mathbf{y}_{n+1}=\mathbf{y}_n+\Delta t[\alpha\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+(1-\alpha)\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)$ $+\beta\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1})+(1-\beta)\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)]$.	IIE1
$k=2$	$\mathbf{y}_{n+1}+a_0\mathbf{y}_n+a_1\mathbf{y}_{n-1}=\Delta t\left(b_{-1}^{[1]}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[1]}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+b_1^{[1]}\mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})\right)$ $+\Delta t\left(b_{-1}^{[2]}\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[2]}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+b_1^{[2]}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})\right)$ $+\Delta t\left(b_0^{[3]}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)+b_1^{[3]}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1})\right)$.	IIE2
$k=3$	$\mathbf{y}_{n+1}+a_0\mathbf{y}_n+a_1\mathbf{y}_{n-1}+a_2\mathbf{y}_{n-2}=$ $\Delta t\left(b_{-1}^{[1]}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[1]}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+b_1^{[1]}\mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[1]}\mathbf{f}^{[1]}(t_{n-2},\mathbf{y}_{n-2})\right)$ $+\Delta t\left(b_{-1}^{[2]}\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[2]}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+b_1^{[2]}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[2]}\mathbf{f}^{[2]}(t_{n-2},\mathbf{y}_{n-2})\right)$ $+\Delta t\left(b_0^{[3]}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)+b_1^{[3]}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[3]}\mathbf{f}^{[3]}(t_{n-2},\mathbf{y}_{n-2})\right)$.	IIE3
$k=4$	$\mathbf{y}_{n+1}+a_0\mathbf{y}_n+a_1\mathbf{y}_{n-1}+a_2\mathbf{y}_{n-2}+a_3\mathbf{y}_{n-3}=$ $\Delta t\left(b_{-1}^{[1]}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[1]}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+b_1^{[1]}\mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[1]}\mathbf{f}^{[1]}(t_{n-2},\mathbf{y}_{n-2})+b_3^{[1]}\mathbf{f}^{[1]}(t_{n-3},\mathbf{y}_{n-3})\right)$ $+\Delta t\left(b_{-1}^{[2]}\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[2]}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+b_1^{[2]}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[2]}\mathbf{f}^{[2]}(t_{n-2},\mathbf{y}_{n-2})+b_3^{[2]}\mathbf{f}^{[2]}(t_{n-3},\mathbf{y}_{n-3})\right)$ $+\Delta t\left(b_0^{[3]}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)+b_1^{[3]}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[3]}\mathbf{f}^{[3]}(t_{n-2},\mathbf{y}_{n-2})+b_3^{[3]}\mathbf{f}^{[3]}(t_{n-3},\mathbf{y}_{n-3})\right)$.	IIE4

For simplicity, the stability region can be defined as a region of the parameters $(z_1, z_2, z_3) = (-\mu^2\Delta t, \nu\Delta t, \lambda\Delta t)$. The choice $(\alpha, \beta) = (\frac{1}{2}, \frac{3}{2})$ in IIE1 yields the IIE method

$$\mathbf{y}_{n+1}=\mathbf{y}_n+\Delta t\left[\frac{1}{2}\left(\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)\right)\right. \left.+\frac{1}{2}\left(3\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1})+\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)\right)+\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)\right], \tag{17}$$

which turns out to have favorable stability properties. We refer to this method as IIE-1. We discuss the following cases of stability for the method (17).

- Case 1 (diffusive reaction term $\lambda = -\mu^2$)
  The stability function (16) is given by
  $$\xi(z_1, z_2) = 1 + \frac{iz_2 + 2z_1}{1 - 2z_1}.$$
  The stability region for this case is presented in Table 2, and it can be shown that the method is A_0-stable.
- Case 2 (non-diffusive reaction term $\lambda = i\nu$)
  The stability function (16) is given by
  $$\xi(z_1, z_2) = 1 + \frac{4iz_2 + 2z_1}{2 - z_1 - 3iz_2}.$$
  The stability region for this case is presented in Table 2, and it can be shown that the method is A-stable.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability function (16) is given by
  $$\xi(z_1, z_2) = 1 + \frac{4iz_2 + 4z_1}{2 - 4z_1 - 3iz_2}.$$
  The stability region for this case is presented in Table 2, and it can be shown that the method is A-stable; Table 2.

In addition, we compare the stability of the first-order IIE1 method (17) with the stability of IMEX1 method,

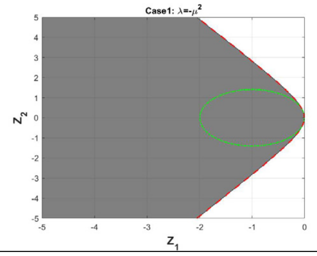
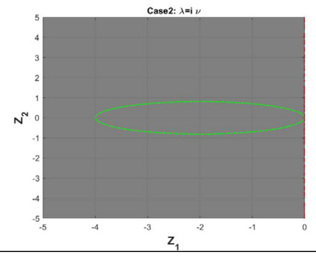
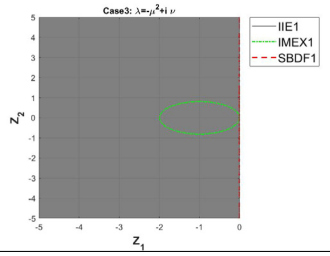
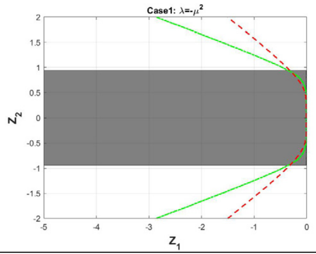
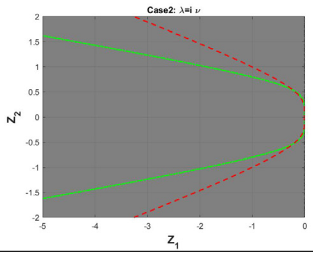
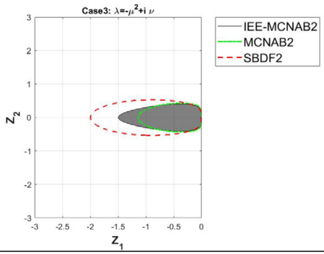
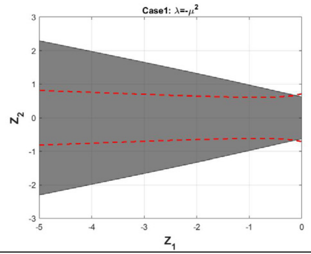
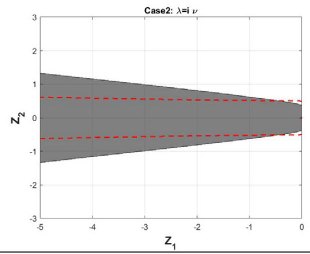
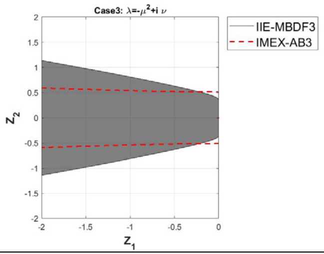
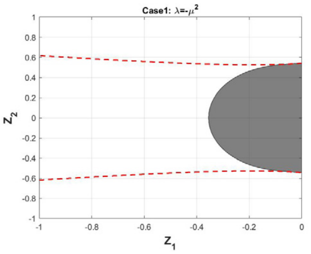
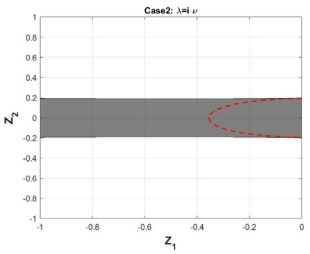
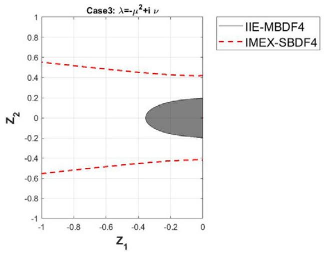
$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{\Delta t}{4}\left(\mathbf{g}(t_{n+1}, \mathbf{y}_{n+1}) + 3\mathbf{g}(t_n, \mathbf{y}_n)\right) + \Delta t\mathbf{f}(t_n, \mathbf{y}_n), \tag{18}$$

and the semi-implicit BDF (SBDF1),

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t\left(\mathbf{g}(t_{n+1}, \mathbf{y}_{n+1}) + \mathbf{f}(t_n, \mathbf{y}_n)\right). \tag{19}$$

It can be noted from Table 2 that the stability region for IIE1 method (17) is significantly larger than the one for SBDF1.

Table 2
Stability regions for IIE-LMMs.

<table>
<tr><th>P</th><th>Case 1: $\lambda = -\mu^2$</th><th>Case 2: $\lambda = i\nu$</th><th>Case 3: $\lambda = -\mu^2 + i\nu$</th></tr>
<tr><td>$P = 1$</td><td></td><td></td><td></td></tr>
<tr><td>$P = 2$</td><td></td><td></td><td></td></tr>
<tr><td>$P = 3$</td><td></td><td></td><td></td></tr>
<tr><td>$P = 4$</td><td></td><td></td><td></td></tr>
</table>

3.1. Two-step, second-order IIE-LMMs

Two-step IIE-LMMs for IVP (1) is presented in Table 1. A second-order method is obtained provided the IIE2 order conditions in Table A.5 are satisfied.

Stability analysis for $k = p = 2$ IIE-LMMs

The second-degree characteristic polynomial resulting from (IIE2) applied to the test equation (14) is given by

$$\begin{aligned}\Phi(\xi) \equiv \Big[1 + b_{-1}^{[1]}\Delta t\mu^2 - \Delta t b_{-1}^{[2]}(\lambda_r + i\lambda_i)\Big]\xi^2 \\ + \Big[a_0 - i\Delta t(b_0^{[2]}\lambda_i + b_0^{[3]}\nu) + \Delta t(b_0^{[1]}\mu^2 - b_0^{[2]}\lambda_r)\Big]\xi \\ + a_1 - i\Delta t(b_1^{[2]}\lambda_i + b_1^{[3]}\nu) + \Delta t(b_1^{[1]}\mu^2 - b_1^{[2]}\lambda_r) = 0.\end{aligned}$$

IIE-CNLF method

A two-step, second-order IIE-LMM can be obtained by applying something similar to the Crank–Nicolson leapfrog (CNLF) method for the implicit terms $f^{[1]}(t_{n+1},\mathbf{y}_{n+1})$ and $f^{[2]}(t_{n+1},\mathbf{y}_{n+1})$ and the leapfrog method for the explicit term $f^{[3]}(t_n,\mathbf{y}_n)$ as follows

$$\begin{aligned}\mathbf{y}_{n+1} = \mathbf{y}_{n-1} &+ \Delta t\left(\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1}) + \mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})\right)\\ &+ 2\Delta t\left(\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1}) - \mathbf{f}^{[2]}(t_n,\mathbf{y}_n) + \mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})\right) + 2\Delta t\left(\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)\right).\end{aligned} \tag{20}$$

We refer this method to as IIE-CNLF2.

Stability analysis

We discuss the stability of the IIE-CNLF2 method (20) for three cases.

- Case 1 (diffusive reaction term $\lambda = -\mu^2$)
  The stability region for this case is presented in Table 2, and it can be shown that the method is A_0-stable.
- Case 2 (non-diffusive reaction term $\lambda = i\nu$)
  The stability region for this case is presented in Table 2, and it can be shown that the method is A-stable.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability region is presented in Table 2, and it can be shown that the method is A_0-stable with a band of linear stability around the negative real axis that is larger than that of Case 1.

In addition, we compare the stability of IIE-CNLF2 method (20) with the stability of the second-order IMEX Modified CNAB (MCNAB2) method,

$$\begin{aligned}\mathbf{y}_{n+1} = \mathbf{y}_n &+ \Delta t\left(\frac{9}{16}\mathbf{g}(t_{n+1},\mathbf{y}_{n+1}) + \frac{3}{8}\mathbf{g}(t_n,\mathbf{y}_n) + \frac{1}{16}\mathbf{g}(t_{n-1},\mathbf{y}_{n-1})\right)\\ &+ \Delta t\left(\frac{3}{2}\mathbf{f}(t_n,\mathbf{y}_n) - \frac{1}{2}\mathbf{f}(t_{n-1},\mathbf{y}_{n-1})\right),\end{aligned} \tag{21}$$

and the SBDF2 method,

$$\mathbf{y}_{n+1} = \frac{4}{3}\mathbf{y}_n - \frac{1}{3}\mathbf{y}_{n-1} + \frac{2}{3}\Delta t\left(\mathbf{g}(t_{n+1},\mathbf{y}_{n+1})\right) + \Delta t\left(\frac{4}{3}\mathbf{f}(t_n,\mathbf{y}_n) - \frac{2}{3}\mathbf{f}(t_{n-1},\mathbf{y}_{n-1})\right). \tag{22}$$

It can be noted from Table 2 that the stability region for IIE-CNLF2 method (20) is significantly larger than the stability regions for MCNAB2 and SBDF2 methods for the case $\lambda = i\nu$.

3.2. Three-step, third-order IIE-LMMs

Three-step IIE-LMMs for IVP (1) is presented Table 1. A third-order method is obtained provided the IIE3 order conditions in Table A.5 are satisfied.

Stability analysis for $k = p = 3$ IIE-LMMs

The third-degree characteristic polynomial resulting from (IIE2) applied to the test equation (14) is given by

$$\begin{aligned}\Phi(\xi) \equiv &\left[1 + b_{-1}^{[1]}\Delta t\mu^2 - \Delta t b_{-1}^{[2]}(\lambda_r + i\lambda_i)\right]\xi^3\\ &+ \left[a_0 - i\Delta t(b_0^{[2]}\lambda_i + b_0^{[3]}\nu) + \Delta t(\mu^2 b_0^{[1]} - b_0^{[2]}\lambda_r)\right]\xi^2\\ &+ \left[a_1 - i\Delta t(b_1^{[2]}\lambda_i + b_1^{[3]}\nu) + \Delta t(\mu^2 b_1^{[1]} - b_1^{[2]}\lambda_r)\right]\xi\\ &+ \left[a_2 - i\Delta t(b_2^{[2]}\lambda_i + b_2^{[3]}\nu) + \Delta t(\mu^2 b_2^{[1]} - b_2^{[2]}\lambda_r)\right] = 0.\end{aligned}$$

IIE-MBDF3

A three-step, third-order method can be derived as follows

$$
\begin{aligned}
\mathbf{y}_{n+1} - \frac{18}{11}\mathbf{y}_n + \frac{9}{11}\mathbf{y}_{n-1} - \frac{2}{11}\mathbf{y}_{n-2} &= \Delta t\left(\frac{6}{11}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})\right) \\
&+ \Delta t\left(\frac{1}{2}\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1}) + \frac{3}{22}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n) - \frac{3}{22}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1}) + \frac{1}{22}\mathbf{f}^{[2]}(t_{n-2},\mathbf{y}_{n-2})\right) \\
&+ \Delta t\left(\frac{18}{11}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n) - \frac{18}{11}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1}) + \frac{6}{11}\mathbf{f}^{[3]}(t_{n-2},\mathbf{y}_{n-2})\right).
\end{aligned} \tag{23}
$$

Because this method applies the third-order BDF method for the implicit term, we refer this method to IIE-MBDF3 (modified third-order BDF).

Stability analysis

We discuss the stability of the IIE-MBDF3 method (23) for three cases.

- Case 1 (diffusive reaction term $\lambda = -\mu^2$)
  The stability region for the method (23) is presented in Table 2, and it can be shown that the method is A_0-stable.
- Case 2 (non-diffusive reaction term $\lambda = i\nu$)
  The stability region for the method (23) is presented in Table 2, and it can be shown that the method is A_0-stable.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability region for the method (23) is presented in Table 2, and it can be shown that the method is A_0-stable.

In addition, we compare the stability of IIE-MBDF3 method (23) with the stability of IMEX Adams–Bashforth (IMEX-AB3) method,

$$
\begin{aligned}
\mathbf{y}_{n+1} = \mathbf{y}_n &+ \Delta t\left(\frac{4661}{10000}\mathbf{g}(t_{n+1},\mathbf{y}_{n+1}) + \frac{324}{625}\mathbf{g}(t_n,\mathbf{y}_n) + \frac{13}{200}\mathbf{g}(t_{n-1},\mathbf{y}_{n-1}) - \frac{247}{5000}\mathbf{g}(t_{n-2},\mathbf{y}_{n-2})\right) \\
&+ \Delta t\left(\frac{23}{12}\mathbf{f}(t_n,\mathbf{y}_n) - \frac{4}{3}\mathbf{f}(t_{n-1},\mathbf{y}_{n-1}) + \frac{5}{12}\mathbf{f}(t_{n-2},\mathbf{y}_{n-2})\right).
\end{aligned} \tag{24}
$$

It can be noted from Table 2 that the stability region for the IIE-MBDF3 method (23) is larger than that of the IMEX-AB3 method.

3.3. Four-step, fourth-order IIE-LMMs

Four-step IIE-LMMs for (1) is presented in Table 1. A fourth-order method is obtained provided the IIE4 order conditions in Table A.5 are satisfied.

Stability analysis for $k = p = 4$ IIE-LMMs

The fourth-degree characteristic polynomial resulting from (IIE2) applied to the test equation (14) is given by

$$
\begin{aligned}
\Phi(\xi) \equiv &\left[1 + b_{-1}^{[1]}\Delta t\mu^2 - \Delta t b_{-1}^{[2]}(\lambda_r + i\lambda_i)\right]\xi^4 \\
&+ \left[a_0 - i\Delta t(b_0^{[2]}\lambda_i + b_0^{[3]}\nu) + \Delta t(\mu^2 b_0^{[1]} - b_0^{[2]}\lambda_r)\right]\xi^3 \\
&+ \left[a_1 - i\Delta t(b_1^{[2]}\lambda_i + b_1^{[3]}\nu) + \Delta t(\mu^2 b_1^{[1]} - b_1^{[2]}\lambda_r)\right]\xi^2 \\
&+ \left[a_2 - i\Delta t(b_2^{[2]}\lambda_i + b_2^{[3]}\nu) + \Delta t(\mu^2 b_2^{[1]} - b_2^{[2]}\lambda_r)\right]\xi \\
&+ \left[a_3 - i\Delta t(b_3^{[2]}\lambda_i + b_3^{[3]}\nu) + \Delta t(\mu^2 b_3^{[1]} - b_3^{[2]}\lambda_r)\right] = 0.
\end{aligned}
$$

IIE-MBDF4

A four-step, fourth-order method can be obtained by applying the fourth-order BDF method for the implicit terms as follows

$$
\begin{aligned}
&\mathbf{y}_{n+1} - \frac{48}{25}\mathbf{y}_n + \frac{36}{25}\mathbf{y}_{n-1} - \frac{16}{25}\mathbf{y}_{n-2} + \frac{3}{25}\mathbf{y}_{n-3} \\
&\quad = \Delta t\left(\frac{12}{25}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})\right) - \Delta t\left(\frac{12}{25}\mathbf{f}^{[2]}(t_{n+1},\mathbf{y}_{n+1}) - \frac{96}{25}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)\right. \\
&\qquad\qquad \left. + \frac{144}{25}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1}) - \frac{96}{25}\mathbf{f}^{[2]}(t_{n-2},\mathbf{y}_{n-2}) + \frac{24}{25}\mathbf{f}^{[2]}(t_{n-3},\mathbf{y}_{n-3})\right) \\
&\qquad + \Delta t\left(\frac{48}{25}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n) - \frac{72}{25}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1}) + \frac{48}{25}\mathbf{f}^{[3]}(t_{n-2},\mathbf{y}_{n-2}) - \frac{12}{25}\mathbf{f}^{[3]}(t_{n-3},\mathbf{y}_{n-3})\right).
\end{aligned} \tag{25}
$$

We refer this method to IIE-MBDF4. We discuss the stability of the IIE-MBDF4 method (25) for three cases.

- Case 1: (diffusive reaction term $\lambda = -\mu^2$)
  The stability region for the method (25) is presented in Table 2, where we see a relatively small linear stability region.
- Case 2: (non-diffusive reaction term $\lambda = i\nu$)
  The stability region for the method (25) in this case is presented in Table 2, and it can be shown that the method is A_0-stable.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability region for the method (25) in this case is presented in Table 2, where we see a relatively small region even compared to that of Case 1.

In summary, we get A-stability in many situations for first and second-order IIE-LMMs and A_0-stability for the second, third, and fourth-order IIE-LMMs. Accordingly, second- and third-order IIE-LMMs could be highly suitable choices for DRA problems that suffer from time step size restrictions due to stability. In addition, we compare the IIE-MBDF4 method (25) with the fourth-order IMEX-SBDF4 method,

$$
\begin{aligned}
\mathbf{y}_{n+1} =& \frac{48}{25}\mathbf{y}_n - \frac{36}{25}\mathbf{y}_{n-1} + \frac{16}{25}\mathbf{y}_{n-2} - \frac{3}{25}\mathbf{y}_{n-3} + \Delta t\left(\frac{12}{25}\mathbf{g}(t_{n+1},\mathbf{y}_{n+1})\right) \\
&+ \Delta t\left(\frac{48}{25}\mathbf{f}(t_n,\mathbf{y}_n) - \frac{72}{25}\mathbf{f}(t_{n-1},\mathbf{y}_{n-1}) + \frac{48}{25}\mathbf{f}(t_{n-2},\mathbf{y}_{n-2}) - \frac{12}{25}\mathbf{f}(t_{n-3},\mathbf{y}_{n-3})\right).
\end{aligned} \tag{26}
$$

It can be noted from Table 2 that the stability region for the IIE-MBDF4 method (25) is larger than the stability region of the IMEX-SBDF4 method for the case $\lambda = i\nu$.

4. *k*-step IEE linear multistep methods

In the ODE (1), if the implicit method is applied to $\mathbf{f}^{[1]}(t,\mathbf{y})$, whereas the explicit methods are applied to $\mathbf{f}^{[2]}(t,\mathbf{y})$ and $\mathbf{f}^{[3]}(t,\mathbf{y})$, then k-step IEE-LMMs for (1) can be written as

$$
\begin{aligned}
\frac{1}{\Delta t}\mathbf{y}_{n+1} + \frac{1}{\Delta t}\sum_{j=0}^{k-1} a_j\mathbf{y}_{n-j} = & \sum_{j=-1}^{k-1} b_j^{[1]}\mathbf{f}^{[1]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=0}^{k-1} b_j^{[2]}\mathbf{f}^{[2]}(t_{n-j},\mathbf{y}_{n-j}) \\
& + \sum_{j=0}^{k-1} b_j^{[3]}\mathbf{f}^{[3]}(t_{n-j},\mathbf{y}_{n-j}),
\end{aligned} \tag{27}
$$

where we assume that $b_{-1}^{[1]} \neq 0$. Expanding (27) in a Taylor series about t_n to obtain the truncation error yields

$$
\begin{aligned}
1 + \sum_{j=0}^{k-1} a_j &= 0, \\
1 - \sum_{j=1}^{k-1} j a_j &= \sum_{j=-1}^{k-1} b_j^{[1]} = \sum_{j=0}^{k-1} b_j^{[2]} = \sum_{j=0}^{k-1} b_j^{[3]}, \\
\frac{1}{2} + \sum_{j=1}^{k-1} \frac{j^2}{2} a_j &= b_{-1}^{[1]} - \sum_{j=1}^{k-1} j b_j^{[1]} = -\sum_{j=1}^{k-1} j b_j^{[2]} = -\sum_{j=1}^{k-1} j b_j^{[3]}, \\
&\vdots
\end{aligned} \tag{28}
$$

$$\frac{1}{p!}+\sum_{j=1}^{k-1}\frac{(-j)^p}{p!}a_j=\frac{b_{-1}^{[1]}}{(p-1)!}+\sum_{j=1}^{k-1}\frac{(-j)^{p-1}b_j^{[1]}}{(p-1)!}=\sum_{j=1}^{k-1}\frac{(-j)^{p-1}b_j^{[2]}}{(p-1)!}=\sum_{j=1}^{k-1}\frac{(-j)^{p-1}b_j^{[3]}}{(p-1)!}.$$

Similar to the argument in section 3, one can prove the following theorem.

Theorem 2. *For the k-step IEE-LMMs (27), we have:*

I. If $p \le k$, then the $3p+1$ conditions of the system (28) are linearly independent. So there exist k-step IEE-LMMs of order k.
II. The order of accuracy of a k-step LMM is at most k.
III. The family of k-step IEE-LMM of order k has k free parameters.

Corollary 1. *Any k-step IEE-LMM of order k reduces to an IMEX-LMM.*

Proof. Assume the k-step IEE-LMM has order k; then we have

$$\begin{aligned}\sum_{j=0}^{k-1}b_j^{[2]}&=\sum_{j=0}^{k-1}b_j^{[3]},\\ \sum_{j=1}^{k-1}(-j)b_j^{[2]}&=\sum_{j=1}^{k-1}(-j)b_j^{[3]},\\ &\vdots\\ \sum_{j=1}^{k-1}(-j)^{k-1}b_j^{[2]}&=\sum_{j=1}^{k-1}(-j)^{k-1}b_j^{[3]}.\end{aligned}\tag{29}$$

Let $\mu_j=b_j^{[2]}-b_j^{[3]}$, then the system (29) is written as

$$\begin{aligned}\sum_{j=0}^{k-1}\mu_j&=0,\\ \sum_{j=1}^{k-1}(-j)\mu_j&=0,\\ &\vdots\\ \sum_{j=1}^{k-1}(-j)^{k-1}\mu_j&=0.\end{aligned}\tag{30}$$

Writing the system (30) in a matrix form yields

$$\begin{bmatrix}1 & 1 & \dots & 1 & \\ 0 & -1 & \dots & 1-k & \\ \vdots & \vdots & \vdots & \dots & \vdots\\ 0 & (-1)^k & \dots & (1-k)^k & \end{bmatrix}_{k\times k}\begin{bmatrix}\mu_0\\ \mu_1\\ \vdots\\ \mu_{k-1}\end{bmatrix}_{k\times 1}=\mathbf{0},$$

implying that $b_j^{[2]}=b_j^{[3]}$, $j=1,2,\dots,k-1$, because the matrix of coefficient is nonsingular. So the method is IMEX-LMM. □

Therefore, we restrict the analysis to k-step IEE-LMMs of order $p=k-1$.

4.1. Linear stability analysis for IEE-LMMs

Consider the scalar test problem (14). Applying IEE-LMM (27) to (14) yields

$$\left[1+\Delta t b_{-1}^{[1]}\mu^2\right]y_{n+1}+\sum_{j=0}^{k-1}\left[a_j-i\Delta t(b_j^{[2]}\lambda_i+b_j^{[3]}\nu)+\Delta t(b_j^{[1]}\mu^2-b_j^{[2]}\lambda_r)\right]y_{n-j}=0.$$

Table 3
IEE-LMMs.

k	Methods	
$k=2$	$\mathbf{y}_{n+1}+a_0\mathbf{y}_n+a_1\mathbf{y}_{n-1}=\Delta t\left(b_{-1}^{[1]}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[1]}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+b_1^{[1]}\mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})\right)+$ $\Delta t\left(b_0^{[2]}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+b_1^{[2]}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})\right)+\Delta t\left(b_0^{[3]}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)+b_1^{[3]}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1})\right).$	IEE2
$k=3$	$\mathbf{y}_{n+1}+a_0\mathbf{y}_n+a_1\mathbf{y}_{n-1}+a_2\mathbf{y}_{n-2}=$ $\Delta t\left(b_{-1}^{[1]}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[1]}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+b_1^{[1]}\mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[1]}\mathbf{f}^{[1]}(t_{n-2},\mathbf{y}_{n-2})\right)+$ $\Delta t\left(b_0^{[2]}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+b_1^{[2]}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[2]}\mathbf{f}^{[2]}(t_{n-2},\mathbf{y}_{n-2})\right)+$ $\Delta t\left(b_0^{[3]}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)+b_1^{[3]}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[3]}\mathbf{f}^{[3]}(t_{n-2},\mathbf{y}_{n-2})\right).$	IEE3
$k=4$	$\mathbf{y}_{n+1}+a_0\mathbf{y}_n+a_1\mathbf{y}_{n-1}+a_2\mathbf{y}_{n-2}+a_3\mathbf{y}_{n-3}=$ $\Delta t\left(b_{-1}^{[1]}\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+b_0^{[1]}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+b_1^{[1]}\mathbf{f}^{[1]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[1]}\mathbf{f}^{[1]}(t_{n-2},\mathbf{y}_{n-2})+b_3^{[1]}\mathbf{f}^{[1]}(t_{n-3},\mathbf{y}_{n-3})\right)$ $+\Delta t\left(b_0^{[2]}\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+b_1^{[2]}\mathbf{f}^{[2]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[2]}\mathbf{f}^{[2]}(t_{n-2},\mathbf{y}_{n-2})+b_3^{[2]}\mathbf{f}^{[2]}(t_{n-3},\mathbf{y}_{n-3})\right)$ $+\Delta t\left(b_0^{[3]}\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)+b_1^{[3]}\mathbf{f}^{[3]}(t_{n-1},\mathbf{y}_{n-1})+b_2^{[3]}\mathbf{f}^{[3]}(t_{n-2},\mathbf{y}_{n-2})+b_3^{[3]}\mathbf{f}^{[3]}(t_{n-3},\mathbf{y}_{n-3})\right).$	IEE4

If this linear constant-coefficient difference equation has solutions of the form $\mathbf{y}_n=\xi^n$, then the characteristic equation is given by

$$\Phi(\xi)\equiv\left[1+b_{-1}^{[1]}\Delta t\mu^2\right]\xi^k+\sum_{j=0}^{k-1}\left[a_j-i\Delta t(b_j^{[2]}\lambda_i+b_j^{[3]}\nu)+\Delta t(b_j^{[1]}\mu^2-b_j^{[2]}\lambda_r)\right]\xi^{k-j-1}. \tag{31}$$

Similar to analysis in section 3, we discuss the stability of IEE-LMMs in three cases $\lambda=i\nu$, $\lambda=-\mu^2$ and $\lambda=-\mu^2+i\nu$.

5. Construction and stability of IEE-LMMs

In this section, we construct IEE-LMMs by using the coefficients of well-known IMEX methods for the $\mathbf{f}^{[1]}$ (diffusion) and $\mathbf{f}^{[3]}$ (advection) terms, and then derive coefficients of $\mathbf{f}^{[2]}$ (reaction) terms that satisfy the relevant order conditions (28). The order conditions for IEE-LMMs methods are summarized in Table A.6. We then also analyze the linear stability of the constructed methods using eq. (14) in the three cases described. The linear stability regions for IEE-LMMs up to fourth order are presented in Table 4.

One-step, first-order IEE-LMMs

The first-order IEE-LMMs for the IVP (1) can be written as

$$\mathbf{y}_{n+1}=\mathbf{y}_n+\Delta t\left[\alpha\mathbf{f}^{[1]}(t_{n+1},\mathbf{y}_{n+1})+\beta\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+\gamma\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)\right]. \tag{32}$$

For a smooth function $\mathbf{y}(t)$, we expand (32) in a Taylor series about $t_n=n\Delta t$ to obtain the truncation error. This yields

$$\begin{aligned}\mathbf{y}_n+\Delta t\dot{\mathbf{y}}_n+\frac{(\Delta t)^2}{2}\ddot{\mathbf{y}}_n+\cdots=&\,\mathbf{y}_n+\Delta t\alpha\left[\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)+\Delta t\frac{\mathrm{d}\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)}{\mathrm{d}t}+\frac{(\Delta t)^2}{2}\frac{\mathrm{d}^2\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)}{\mathrm{d}t^2}+\dots\right]\\&+\Delta t\beta\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)+\Delta t\gamma\mathbf{f}^{[3]}(t_n,\mathbf{y}_n).\end{aligned} \tag{33}$$

Applying (1) to the truncation error (33) provides:

- Coefficients of $\mathbf{f}^{[1]}(t_n,\mathbf{y}_n)$: $\Delta t(1-\alpha)=0$, implying that $\alpha=1$.
- Coefficients of $\mathbf{f}^{[2]}(t_n,\mathbf{y}_n)$: $\Delta t(1-\beta)=0$, implying that $\beta=1$.
- Coefficients of $\mathbf{f}^{[3]}(t_n,\mathbf{y}_n)$: $\Delta t(1-\gamma)=0$, implying that $\gamma=1$.

Therefore, the method (32) turns into an IMEX method, in agreement with the result of Corollary 1.

Two-step, first-order IEE-LMMs

Two-step IEE-LMMs for IVP (1) is presented in Table 3. A first-order method is obtained provided the IEE2 order conditions in Table A.6 are satisfied.

Stability analysis for two-step, first-order IEE-LMMs

The second-degree characteristic polynomial resulting from IEE2 applied to the test equation (14) is given by

$$\Phi(\xi) \equiv \left[1 + b_{-1}^{[1]}\Delta t\mu^2\right]\xi^2 + \left[a_0 - i\Delta t(b_0^{[2]}\lambda_i + b_0^{[3]}\nu) + \Delta t(b_0^{[1]}\mu^2 - b_0^{[2]}\lambda_r)\right]\xi$$
$$+ a_1 - i\Delta t(b_1^{[2]}\lambda_i + b_1^{[3]}\nu) + \Delta t(b_1^{[1]}\mu^2 - b_1^{[2]}\lambda_r) = 0.$$

IEE-MCNAB1 method

A two-step, first-order IEE-LMM can be obtained by applying something similar to the Crank–Nicolson (CN) method for the implicit term $\mathbf{f}^{[1]}(t_{n+1}, \mathbf{y}_{n+1})$, the second-order Adams–Bashforth (AB) method for the explicit term $\mathbf{f}^{[3]}(t_n, \mathbf{y}_n)$, and a method for $\mathbf{f}^{[2]}(t_n, \mathbf{y}_n)$ derived from the solution of the IEE2 order conditions as follows:

$$\begin{aligned}\mathbf{y}_{n+1} = \mathbf{y}_n &+ \frac{\Delta t}{2}\left(\mathbf{f}^{[1]}(t_{n+1}, \mathbf{y}_{n+1}) + \mathbf{f}^{[1]}(t_n, \mathbf{y}_n)\right) + \frac{\Delta t}{2}\left(\mathbf{f}^{[2]}(t_n, \mathbf{y}_n) + \mathbf{f}^{[2]}(t_{n-1}, \mathbf{y}_{n-1})\right) \\ &+ \frac{\Delta t}{2}\left(3\mathbf{f}^{[3]}(t_n, \mathbf{y}_n) - \mathbf{f}^{[3]}(t_{n-1}, \mathbf{y}_{n-1})\right).\end{aligned} \tag{34}$$

We refer this method to as IEE-MCNAB1 (modified first-order CNAB) method.

Stability analysis

We discuss the stability of the IEE-MCNAB1 method (34) for three cases.

- Case 1: (diffusive reaction term $\lambda = -\mu^2$)
  The stability region for the method (34) is presented in Table 4, and it can be shown that the method is A_0-stable.
- Case 2: (non-diffusive reaction term $\lambda = i\nu$)
  The stability region for the method (34) is presented in Table 4, and it can be shown that the method is A_0-stable and appears to capture the negative real axis better than Case 1.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability region for the method (34) is presented in Table 4. In this case, the method can be shown to be A_0-stable and captures the negative real axis intermediate to Cases 1 and 2.

In addition, we compare the two-step, first-order IEE-MCNAB1 method (34) with the IMEX1 method (18) and the semi-implicit BDF (SBDF1) (19).

Three-step, second-order IEE-LMMs

Three-step IEE-LMMs for IVP (1) are presented in Table 3. A second-order method is obtained provided the IEE3 order conditions in Table A.6 are satisfied.

Stability analysis for three-step, second-order IEE-LMMs

The third-degree characteristic polynomial resulting from IEE3 applied to the test equation (14) is given by

$$\begin{aligned}\Phi(\xi) \equiv &\left[1 + \Delta t b_{-1}^{[1]}\mu^2\right]\xi^3 \\ &+ \left[a_0 - i\Delta t(b_0^{[2]}\lambda_i + b_0^{[3]}\nu) + \Delta t(\mu^2 b_0^{[1]} - b_0^{[2]}\lambda_r)\right]\xi^2 \\ &+ \left[a_1 - i\Delta t(b_1^{[2]}\lambda_i + b_1^{[3]}\nu) + \Delta t(\mu^2 b_1^{[1]} - b_1^{[2]}\lambda_r)\right]\xi \\ &+ \left[a_2 - i\Delta t(b_2^{[2]}\lambda_i + b_2^{[3]}\nu) + \Delta t(\mu^2 b_2^{[1]} - b_2^{[2]}\lambda_r)\right] = 0\end{aligned} \tag{35}$$

IEE-MCNAB2 method

A three-step, second-order method can be derived as follows

$$\begin{aligned}\mathbf{y}_{n+1} - \mathbf{y}_n = &\Delta t\left(\frac{1}{2}\mathbf{f}^{[1]}(t_{n+1}, \mathbf{y}_{n+1}) + \frac{1}{2}\mathbf{f}^{[1]}(t_n, \mathbf{y}_n)\right) \\ &+ \Delta t\left(\frac{3}{2}\mathbf{f}^{[2]}(t_n, \mathbf{y}_n) - \frac{1}{2}\mathbf{f}^{[2]}(t_{n-1}, \mathbf{y}_{n-1})\right) \\ &+ \Delta t\left(\frac{4}{3}\mathbf{f}^{[3]}(t_n, \mathbf{y}_n) - \frac{1}{6}\mathbf{f}^{[3]}(t_{n-1}, \mathbf{y}_{n-1}) - \frac{1}{6}\mathbf{f}^{[3]}(t_{n-2}, \mathbf{y}_{n-2})\right).\end{aligned} \tag{36}$$

This method uses the second-order CN method for the implicit term $\mathbf{f}^{[1]}(t_{n+1}, \mathbf{y}_{n+1})$, the second-order AB for the explicit term $\mathbf{f}^{[2]}(t_n, \mathbf{y}_n)$, and a method for $\mathbf{f}^{[3]}(t_n, \mathbf{y}_n)$ derived from IEE3 order conditions. We refer this method to as IEE-MCNAB2 (modified second-order CNAB).

Stability analysis

We discuss the stability of the IEE-MCNAB2 method (36) for three cases.

- Case 1: (diffusive reaction term $\lambda = -\mu^2$)
  The stability region for the method (36) is presented in Table 4, from where we see the stability region is bounded.
- Case 2: (non-diffusive reaction term $\lambda = i\nu$)
  The stability region for the method (36) is presented in Table 4, from where we see the stability region is smaller than in Case 1.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability region for the method (36) is presented in Table 4, from where we see the size of the stability region is intermediate to Cases 1 and 2.

In addition, we compare the stability region of the IEE-MCNAB2 method (36) with the stability region of the second-order IMEX MCNAB2 method (21) and the SBDF2 method (22).

Four-step, third-order IEE-LMMs

Four-step IEE-LMMs for IVP (1) is presented in Table 3. A third-order method is obtained provided the IEE4 order conditions in Table A.6 are satisfied.

Stability analysis for four-step, third-order IEE-LMMs

The fourth-degree characteristic polynomial resulting from IEE4 applied to the test equation (14) is given by

$$\begin{aligned}\Phi(\xi) \equiv &\left[1 + b_{-1}^{[1]}\Delta t\mu^2\right]\xi^4 \\ &+ \left[a_0 - i\Delta t(b_0^{[2]}\lambda_i + b_0^{[3]}\nu) + \Delta t(\mu^2 b_0^{[1]} - b_0^{[2]}\lambda_r)\right]\xi^3 \\ &+ \left[a_1 - i\Delta t(b_1^{[2]}\lambda_i + b_1^{[3]}\nu) + \Delta t(\mu^2 b_1^{[1]} - b_1^{[2]}\lambda_r)\right]\xi^2 \\ &+ \left[a_2 - i\Delta t(b_2^{[2]}\lambda_i + b_2^{[3]}\nu) + \Delta t(\mu^2 b_2^{[1]} - b_2^{[2]}\lambda_r)\right]\xi \\ &+ \left[a_3 - i\Delta t(b_3^{[2]}\lambda_i + b_3^{[3]}\nu) + \Delta t(\mu^2 b_3^{[1]} - b_3^{[2]}\lambda_r)\right] = 0.\end{aligned}$$

IEE-MBDF3

A four-step, third-order method can be obtained as follows:

$$\begin{aligned}\mathbf{y}_{n+1} - \frac{18}{11}\mathbf{y}_n + \frac{9}{11}\mathbf{y}_{n-1} - \frac{2}{11}\mathbf{y}_{n-2} = {}&\Delta t\left(\frac{6}{11}\mathbf{f}^{[1]}(t_{n+1}, \mathbf{y}_{n+1})\right) + \Delta t\left(\frac{18}{11}\mathbf{f}^{[2]}(t_n, \mathbf{y}_n)\right. \\ &\left. - \frac{18}{11}\mathbf{f}^{[2]}(t_{n-1}, \mathbf{y}_{n-1}) + \frac{6}{11}\mathbf{f}^{[2]}(t_{n-2}, \mathbf{y}_{n-2})\right) \\ &+ \Delta t\left(\frac{47}{22}\mathbf{f}^{[3]}(t_n, \mathbf{y}_n) - \frac{69}{22}\mathbf{f}^{[3]}(t_{n-1}, \mathbf{y}_{n-1})\right. \\ &\left. + \frac{45}{22}\mathbf{f}^{[3]}(t_{n-2}, \mathbf{y}_{n-2}) - \frac{1}{2}\mathbf{f}^{[3]}(t_{n-3}, \mathbf{y}_{n-3})\right).\end{aligned} \tag{37}$$

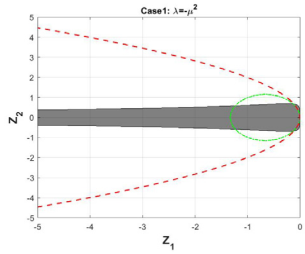
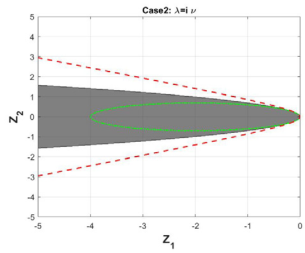
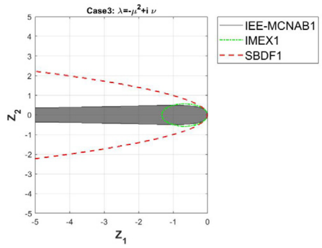
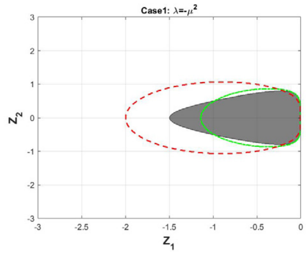
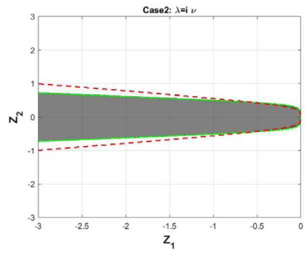
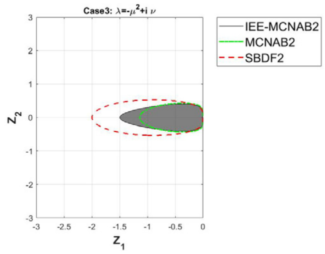
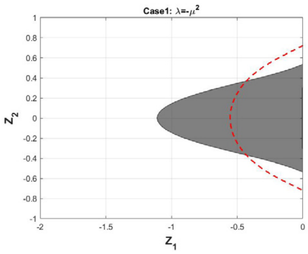
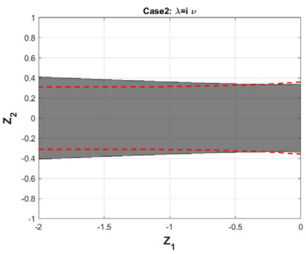
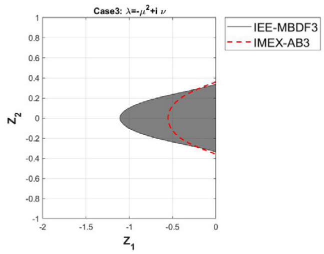
Because this method applies the third-order BDF method for the implicit term, we refer this method to IEE-MBDF3 (modified third-order BDF).

Stability analysis

We discuss the stability of method (37) for three cases

- Case 1: (diffusive reaction term $\lambda = -\mu^2$)
  The stability region for the IEE-MBDF3 method (37) is presented in Table 4, from where we see the stability region is bounded but captures some of the imaginary axis.

Table 4
Stability regions for IEE-LMMs.

k	Case 1: $\lambda = -\mu^2$	Case 2: $\lambda = i\nu$	Case 3: $\lambda = -\mu^2 + i\nu$
$P = 2$			
$P = 3$			
$P = 4$			

- Case 2: (non-diffusive reaction term $\lambda = i\nu$)
  The stability region for the method (37) is presented in Table 4, and it can be shown that the method is A_0-stable.
- Case 3: (mixed reaction term $\lambda = -\mu^2 + i\nu$)
  The stability region for the method (37) is presented in Table 4, where we see a bounded stability region that is smaller than Case 1.

  Finally, we compare the stability region of the IEE-MBDF3 method (37) with the stability region of the IMEX-AB3 method (24).

6. Numerical experiments

In this section, we test the convergence order of the constructed IIE and IEE methods on a spatially discretized non-linear DRA problem. Also, we compare the performance of the 3-additive splitting methods with some well-known IMEX methods on Brusselator DRA model, which is used to describe a reaction-diffusion system with non-linear oscillations [29]. All numerical experiments are performed using MATLAB. Highly accurate starting values for the IIE-LMMs as well as reference solutions for the method-of-lines (MOL) ODEs obtained from spatial discretization of the PDEs are calculated using the variable-stepsize, variable-order solver `ode15s` in MATLAB with an absolute tolerance of 10–14 and a relative tolerance of 2.5 × 10–14.

The nonlinear algebraic equations associated with the implicit methods are solved using a modified Newton's method and the linear systems arising at each Newton iteration are solved using the MATLAB `mldivide` operator (\) [1]. The `mldivide` operator applied to sparse matrices implements a specific direct solver depending on the characteristics of the input matrix. For general sparse matrix, a sparse LU solver is used.

6.1. Order of convergence

To examine the convergence order of the constructed 3-additive methods for solving DRA problems, we consider the nonlinear problem

$$\begin{aligned} &u_t + uu_x = u_{xx} + u + f(x,t),\\ &u(x,0) = \sin(2\pi x),\\ &u(0,t) = u(1,t), \end{aligned} \tag{38}$$

where

$$f(x,t) = \cos(2\pi x + t) + 2\pi \sin(2\pi x + t)\cos(2\pi x + t) + 4\pi^2 \sin(2\pi x + t) - \sin(2\pi x + t)$$

The problem (38) is posed on $t \in [0, 10]$ and $x \in [0, 1]$. We note that the equation (38) is equivalent to $u_t + (\frac{u^2}{2})_x = u_{xx} + u + f(x,t)$. The spatial domain is uniformly discretized into N subintervals with spacing $\Delta x = 1/N$; a second-order centered finite discretization for advection and diffusion terms yields a system of ODEs written as

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = -\left(\frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x}\right) + \left(\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}\right) + u_i + f(i\Delta x, t), \tag{39}$$

where $i = 1, 2, \dots, N$. In this experiment, we also investigate the order of convergence of the methods constructed in section 3 in the maximum norm $\|.\|_\infty$ of errors computed by comparing against a reference solution for equation (39) generated using the `ode15s` solver in MATLAB, at the end point of the interval of integration as a function of the time step. Specifically, we calculate the slope of the line of best fit to the $\log(\|\text{error}\|_\infty)$-$\log(\Delta t)$ data. The results for the constructed 3-additive splitting methods are presented in Fig. 1. We can see that all methods achieve their expected orders of accuracy.

6.2. Performance results

This section compares the performance results of the IIE- and IEE-LMMs introduced in sections 3 and 5 with some popular IMEX splitting methods derived in [34]. The comparisons are made for the following stiff variation of the standard Brusselator problem [14],

$$\begin{aligned} &u_t = \alpha_u \nabla^2 u - \rho_u \nabla u + a - (w+1)u + u^2 v,\\ &v_t = \alpha_v \nabla^2 v - \rho_v \nabla v + wu - u^2 v,\\ &w_t = \alpha_w \nabla^2 w - \rho_w \nabla w + \frac{b-w}{\epsilon} - wu, \end{aligned} \tag{40}$$

solved on $t \in [0, 10]$ and $x \in [0, 1]$ using stationary boundary conditions,

$$u_t(t,0) = u_t(t,1) = v_t(t,0) = v_t(t,1) = w_t(t,0) = w_t(t,1) = 0,$$

and initial values

$$\begin{aligned} &u(0,x) = a + 0.1\sin(\pi x),\\ &v(0,x) = \frac{b}{a} + 0.1\sin(\pi x),\\ &w(0,x) = b + 0.1\sin(\pi x), \end{aligned} \tag{41}$$

with parameters $\alpha_u = \alpha_v = \alpha_w = 10^{-2}$, $\rho_u = \rho_v = \rho_w = 10^{-3}$, $a = 0.6$, $b = 2$, and $\epsilon = 10^{-2}$. The problem (40) is discretized uniformly in space using a second-order accurate centered difference approximation with 100 grid points. The right-hand side of problem (40) is split into three terms as

$$\mathbf{f}^{[1]} = \begin{bmatrix} \alpha_u \nabla^2 u \\ \alpha_v \nabla^2 v \\ \alpha_w \nabla^2 w \end{bmatrix}, \ \mathbf{f}^{[2]} = \begin{bmatrix} a - (w+1)u + u^2 v \\ wu - u^2 v \\ \frac{b-w}{\epsilon} - wu \end{bmatrix}, \ \text{and } \mathbf{f}^{[3]} = \begin{bmatrix} -\rho_u \nabla u \\ -\rho_v \nabla v \\ -\rho_w \nabla w \end{bmatrix}. \tag{42}$$

A reference solution for the MOL ODEs arising from the spatial discretization of equation (40) as described is generated using `ode15s` with an absolute tolerance of 10^{-20} and a relative tolerance of 2.5×10^{-14}. The error is measured by the mixed root mean square (MRMS) error [10]

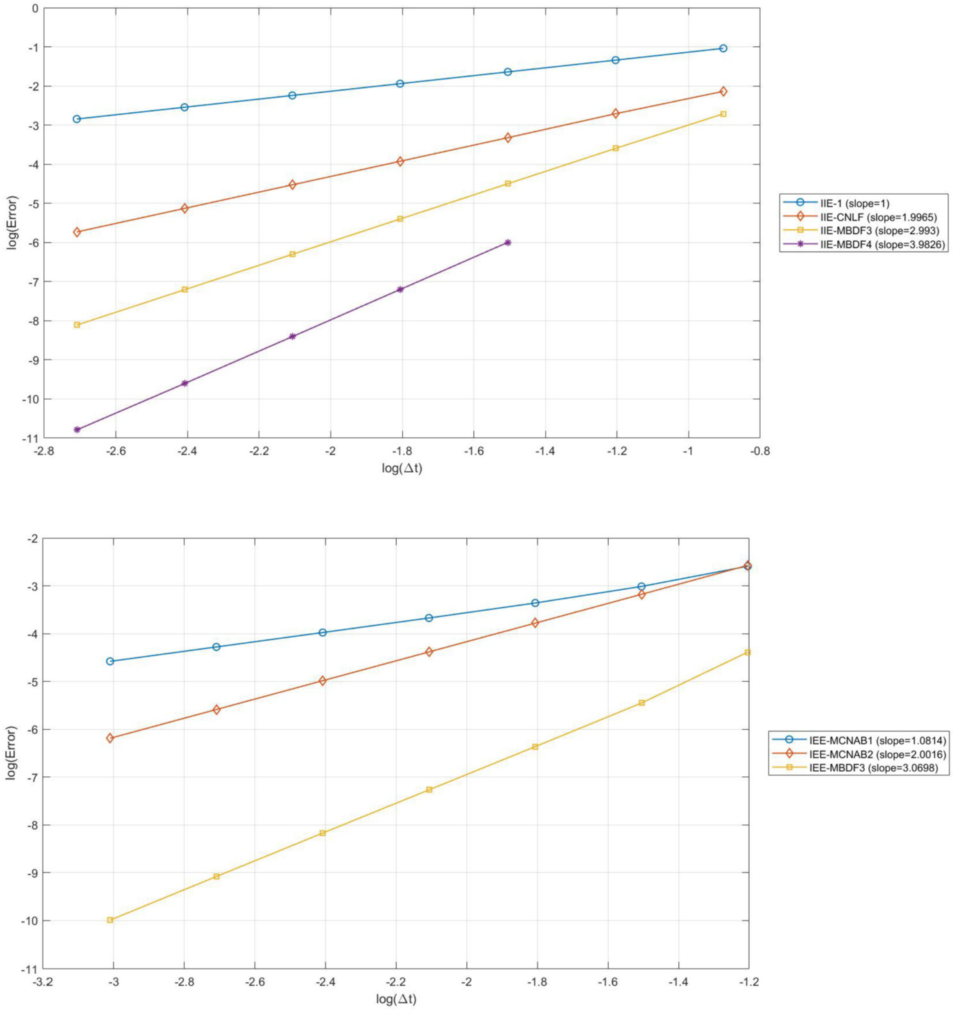


Fig. 1. log-log plot of error vs. time step and line of best fit for DRA equation (39) solved by 3-additive splitting methods.

$$\text{MRMS} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{Y_i - y_i}{1+|Y_i|}\right)^2},$$

where N is the number of solution points, Y_i, and y_i denote the reference and numerical solutions, respectively. Each experiment is performed ten times to mitigate random influences on it; the minimum time measurement of the ten runs is considered because a minimum time gives an indicator of how well a given method performs under ideal conditions. We use a uniform time step size in each experiment, $\Delta t = \frac{2^{-J}}{80}$, $J = 1, 2, \ldots, 5$. Work-precision diagrams are used to compare the performance of the various methods, where the log(MRMS error) of the numerical methods are plotted on the x-axis and the log(CPU time) is plotted on the y-axis.

6.2.1. IIE-LMMs performance results
First-order methods

We compare the first-order IIE1 method (17) with the IMEX1 method (18) and the SBDF1 (19).

Second-order methods

We now compare the IIE-CNLF2 method (20) with the second-order IMEX Modified CNAB (MCNAB2) method (21) and the SBDF2 method (22).

Third-order methods

Here, we compare the IIE-MBDF3 method (23) with the IMEX Adams–Bashforth (IMEX-AB3) method (24).

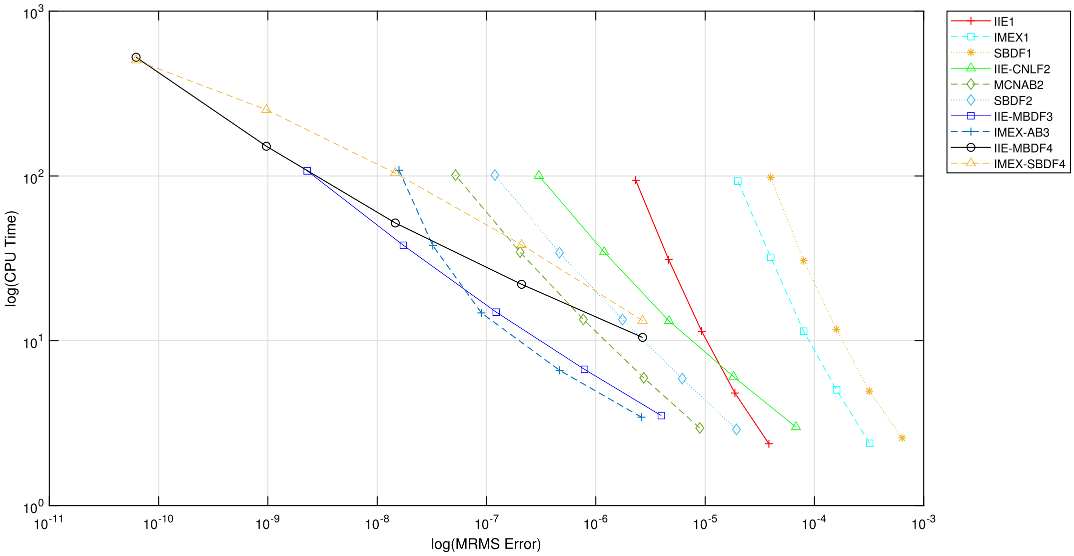


Fig. 2. CPU time versus accuracy.

Fourth-order methods

Finally, we compare the IIE-MBDF4 method (25) with the fourth-order method IMEX-SBDF4 (26).

The work-precision diagram of these methods is given Fig. 2, and it shows that the IIE-MBDF3 and IIE-MBDF4 outperform the other methods tested for small stepsize. The IIE1 significantly outperforms its first-order IMEX counterparts.

6.2.2. IEE-LMMs performance results

First-order methods

We compare the two-step, first-order IEE-MCNAB1 method (34) with the IMEX1 method (18) and the semi-implicit BDF (SBDF) (19).

Second-order methods

We compare the IEE-MCNAB2 method (36) with the second-order IMEX MCNAB2 method (21) and SBDF2 method (22).

Third-order methods

Finally, we compare the IEE-MBDF3 method (37) with the IMEX-AB3 method (24).

The work-precision diagram of these methods is given in Fig. 3, and it shows that the IEE-MBDF3 method outperforms the other methods tested. The IEE-MCNAB2 method outperforms the SBDF2 method and is comparable with the MCNAB2 method.

7. *N*-additive linear multi-step methods

7.1. Extension to $I^{N-1}E$

Consider a differential equation of the form

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t}(t) = \mathbf{f}^{[1]}(t,\mathbf{y}) + \mathbf{f}^{[2]}(t,\mathbf{y}) + \cdots + \mathbf{f}^{[N]}(t,\mathbf{y}). \tag{43}$$

If an implicit method is applied to $\mathbf{f}^{[1]}(t,\mathbf{y}), \mathbf{f}^{[2]}(t,\mathbf{y}), \ldots, \mathbf{f}^{[N-1]}(t,\mathbf{y})$, while an explicit method is applied to $\mathbf{f}^{[N]}(t,\mathbf{y})$, then the k-step I^{N-1}E-LMM can be formulated as:

$$\begin{aligned} \frac{1}{\Delta t}\mathbf{y}_{n+1} + \frac{1}{\Delta t}\sum_{j=0}^{k-1} a_j \mathbf{y}_{n-j} = \sum_{j=-1}^{k-1} b_j^{[1]}\mathbf{f}^{[1]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=-1}^{k-1} b_j^{[2]}\mathbf{f}^{[2]}(t_{n-j},\mathbf{y}_{n-j}) + \ldots \\ + \sum_{j=-1}^{k-1} b_j^{[N-1]}\mathbf{f}^{[N-1]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=0}^{k-1} b_j^{[N]}\mathbf{f}^{[N]}(t_{n-j},\mathbf{y}_{n-j}), \end{aligned} \tag{44}$$

where we assume that $b_{-1}^{[1]}, b_{-1}^{[2]}, \ldots, b_{-1}^{[N-1]} \neq 0$.

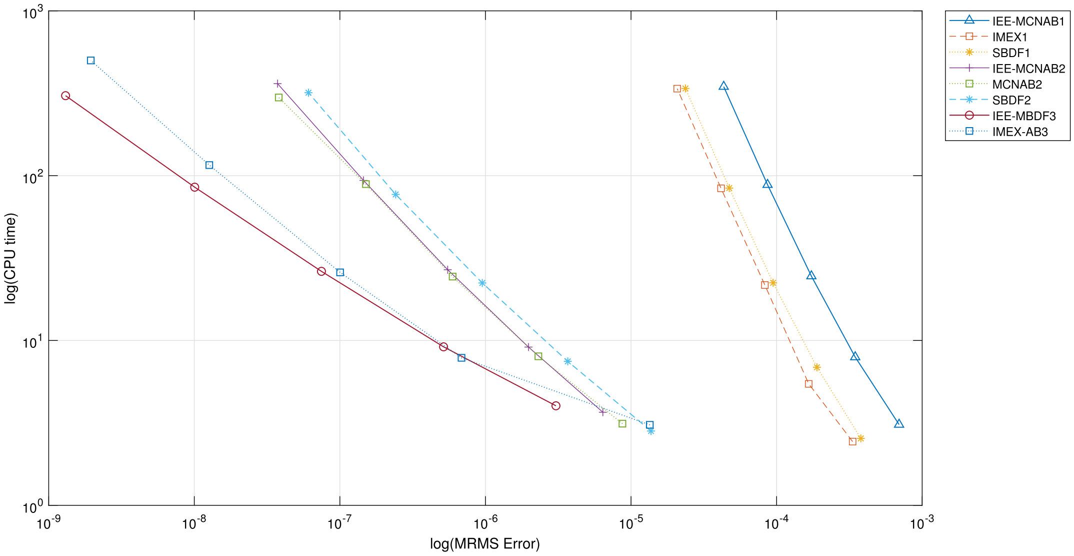


Fig. 3. CPU time versus accuracy.

Order conditions

The order conditions for k-step I^{N-1}E-LMMs can be derived similarly by substituting the exact solution to (43) into (44) and expanding in Taylor series about t_n and analyzing the resulting truncation error. An order-p method is obtained provided

$$\begin{aligned}
&1+\sum_{j=0}^{k-1} a_j = 0,\\
&1-\sum_{j=1}^{k-1} j a_j = \sum_{j=-1}^{k-1} b_j^{[1]} = \cdots = \sum_{j=-1}^{k-1} b_j^{[N-1]} = \sum_{j=0}^{k-1} b_j^{[N]},\\
&\frac{1}{2}+\sum_{j=1}^{k-1}\frac{j^2}{2}a_j = b_{-1}^{[1]} - \sum_{j=1}^{k-1} j b_j^{[1]} = \cdots = b_{-1}^{[N-1]} - \sum_{j=1}^{k-1} j b_j^{[N-1]} = -\sum_{j=1}^{k-1} j b_j^{[N]},\\
&\qquad\vdots\\
&\frac{1}{p!}+\sum_{j=1}^{k-1}\frac{(-j)^p}{p!}a_j = \frac{b_{-1}^{[1]}}{(p-1)!}+\sum_{j=1}^{k-1}\frac{(-j)^{p-1}b_j^{[1]}}{(p-1)!} = \cdots = \frac{b_{-1}^{[N-1]}}{(p-1)!}+\sum_{j=1}^{k-1}\frac{(-j)^{p-1}b_j^{[N-1]}}{(p-1)!} = \sum_{j=1}^{k-1}\frac{(-j)^{p-1}b_j^{[N]}}{(p-1)!}.
\end{aligned} \tag{45}$$

Theorem 3. *For the k-step I^{N-1}E-LMM (44), we have:*

I. If $p \le k$, then the $Np+1$ conditions of the system (45) are linearly independent. So there exist k-step I^{N-1}E methods of order k.
II. The order of accuracy of a k-step I^{N-1}E method is at most k.
III. The family of k-step I^{N-1}E methods of order k has $(N+k-2)$ free parameters.

Proof. I. Because linear independence for $p = k$ implies linear independence for $p \le k$, it is sufficient to prove the case $p = k$ only.

The system (45) can be represented in matrix form

$$\mathbf{W}\mathbf{V} = \mathbf{U},$$

where

$$\mathbf{V} = [a_0, \ldots, a_{k-1}, b_{-1}^{[1]}, b_0^{[1]}, \ldots, b_{k-1}^{[1]}, \ldots, b_{-1}^{[N-1]}, b_0^{[N-1]}, \ldots, b_{k-1}^{[N-1]}, b_0^{[N]}, b_1^{[N]}, \ldots, b_{k-1}^{[N]}]^T \in \mathbb{R}^{(N+1)k+N-1}$$

and

$$\mathbf{U} = [-1, \dots, -1_{k+1}, 0, \dots, 0_{(N-1)k}]^T \in \mathbb{R}^{Nk+1},$$

with the coefficient matrix defined as

$$\mathbf{W} = \left[\begin{array}{cc|c|ccccc} \mathbf{A} & \mathbf{L} & 0 & \dots & 0 & & & \\ \mathbf{H} & & -\mathbf{DA} & \mathbf{0} & \mathbf{0} & & & \\ \hline \mathbf{0} & \mathbf{1} & \mathbf{A} & -\mathbf{1} & -\mathbf{A} & & & \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{A} & -\mathbf{1} & -\mathbf{A} & \\ & & & \ddots & \ddots & \ddots & \ddots & \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} & \mathbf{1} & \mathbf{A} & -\mathbf{1} \quad -\mathbf{A} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & & \mathbf{0} & \mathbf{0} & \mathbf{1} \quad \mathbf{A} \quad -\mathbf{A} \end{array}\right]_{(Nk+1)\times((N+1)k+N-1)},$$

where $\mathbf{A}$, $\mathbf{D}$, $\mathbf{H}$, and $\mathbf{L}$ are defined in (8)–(11), respectively, and $\mathbf{1}$ is a vector of ones with size k.

Because the Vandermonde matrix $\mathbf{A}$ is nonsingular, it can be noted that columns $\{1, k+2, \dots, 2k+1, 2k+3, \dots, 4k+2, \dots, (N-2)k+N-1, \dots, (N-1)k+N-2, (N-1)k+N, \dots, (N+1)k+(N-1)\}$ of the matrix $\mathbf{W}$ are linearly independent. Thus, all $(Np+1)$ conditions are linearly independent and the system (45) admits an $(N(p-k+1)+(p-2))$-parameter family of solutions provided that $p \le k$. Because columns $k+1, 2k+2, \dots, (N-1)k+(N-1)$ of matrix $\mathbf{W}$ do not enter into the proof, $b_{-1}^{[1]}, b_{-1}^{[2]}, \dots, b_{-1}^{[N-1]}$ can have any nonzero value. This property verifies that the family of methods is I^{N-1}E-LMM.

II. Assume the I^{N-1}E-LMM method has accuracy $\mathcal{O}((\Delta t)^{k+r})$, $r \ge 1$; then the following order conditions hold:

$$\begin{aligned} \sum_{j=-1}^{k-1} b_j^{[N-1]} &= \sum_{j=0}^{k-1} b_j^{[N]}, \\ b_{-1}^{[N-1]} + \sum_{j=1}^{k-1}(-j) b_j^{[N-1]} &= \sum_{j=1}^{k-1}(-j) b_j^{[N]}, \\ &\vdots \\ b_{-1}^{[N-1]} + \sum_{j=1}^{k-1}(-j)^k b_j^{[N-1]} &= \sum_{j=1}^{k-1}(-j)^k b_j^{[N]}. \end{aligned} \tag{46}$$

Let $\mu_j = b_j^{[N-1]} - b_j^{[N]}$; then the system (46) can be written as

$$\begin{aligned} b_{-1}^{[N-1]} + \sum_{j=0}^{k-1} \mu_j &= 0, \\ b_{-1}^{[N-1]} + \sum_{j=1}^{k-1}(-j)\mu_j &= 0, \\ &\vdots \\ b_{-1}^{[N-1]} + \sum_{j=1}^{k-1}(-j)^k \mu_j &= 0. \end{aligned} \tag{47}$$

Writing the system (47) in matrix form yields,

$$\begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 0 & -1 & \dots & 1-k \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & 0 & (-1)^k & \dots & (1-k)^k \end{bmatrix}_{(k+1)\times(k+1)} \begin{bmatrix} b_{-1}^{[N-1]} \\ \mu_0 \\ \vdots \\ \mu_{k-1} \end{bmatrix}_{(k+1)\times 1} = \mathbf{0},$$

implying that $b_{-1}^{[N-1]} = 0$ and $b_j^{[N-1]} = b_j^{[N]}$, $j = 1, 2, \dots, k-1$, and contradicting the assumption $b_{-1}^{[N-1]} \neq 0$. So the k-step I^{N-1}E-LMM cannot achieve more than order-k accuracy.

III. Consider the k-step I^{N-1}E-LMM that achieves the highest order of accuracy. Then, as shown above, the family of such method has exactly $(N+k-2)$ free parameters. □

7.2. Extension to IE^{N-1}

Consider a differential equation of the form (43). If an implicit method is applied to $\mathbf{f}^{[1]}(t,\mathbf{y})$, while explicit methods are applied to $\mathbf{f}^{[2]}(t,\mathbf{y}), \mathbf{f}^{[3]}(t,\mathbf{y}), \dots, \mathbf{f}^{[N]}(t,\mathbf{y})$, then the k-step IE^{N-1}-LMM can be formulated as:

$$\begin{aligned}\frac{1}{\Delta t}\mathbf{y}_{n+1} + \frac{1}{\Delta t}\sum_{j=0}^{k-1} a_j \mathbf{y}_{n-j}s = &\sum_{j=-1}^{k-1} b_j^{[1]}\mathbf{f}^{[1]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=0}^{k-1} b_j^{[2]}\mathbf{f}^{[2]}(t_{n-j},\mathbf{y}_{n-j}) + \dots \\ &+ \sum_{j=0}^{k-1} b_j^{[N-1]}\mathbf{f}^{[N-1]}(t_{n-j},\mathbf{y}_{n-j}) + \sum_{j=0}^{k-1} b_j^{[N]}\mathbf{f}^{[N]}(t_{n-j},\mathbf{y}_{n-j}),\end{aligned} \tag{48}$$

where we assume that $b_{-1}^{[1]} \neq 0$ and $b_j^{[1]} \neq b_j^{[2]} \neq \dots \neq b_j^{[N]}$ for some $j \in \{0, 1, \dots, k-1\}$.

Order conditions

The order conditions for k-step IE^{N-1}-LMMs can be derived similarly to analysis of IIE-LMM in section 7.1 by expanding eq. (48) in a Taylor series about t_n and applying eq. (1) to the resulting truncation error. An order-p method is obtained provided

$$\begin{aligned}
&1 + \sum_{j=0}^{k-1} a_j = 0,\\
&1 - \sum_{j=1}^{k-1} j a_j = \sum_{j=-1}^{k-1} b_j^{[1]} = \sum_{j=0}^{k-1} b_j^{[2]} = \dots = \sum_{j=0}^{k-1} b_j^{[N]},\\
&\frac{1}{2} + \sum_{j=1}^{k-1} \frac{j^2}{2} a_j = b_{-1}^{[1]} - \sum_{j=1}^{k-1} j b_j^{[1]} = -\sum_{j=1}^{k-1} j b_j^{[2]} = \dots = -\sum_{j=1}^{k-1} j b_j^{[N]},\\
&\qquad\vdots\\
&\frac{1}{p!} + \sum_{j=1}^{k-1} \frac{(-j)^p}{p!} a_j = \frac{b_{-1}^{[1]}}{(p-1)!} + \sum_{j=1}^{k-1} \frac{(-j)^{p-1} b_j^{[1]}}{(p-1)!} = \sum_{j=1}^{k-1} \frac{(-j)^{p-1} b_j^{[2]}}{(p-1)!} = \dots = \sum_{j=1}^{k-1} \frac{(-j)^{p-1} b_j^{[N]}}{(p-1)!}.
\end{aligned} \tag{49}$$

It is not difficult to generalize Theorem 2 as follows.

Theorem 4. *For the k-step IE^{N-1}-LMM (48), we have:*

I. If $p \le k$, then the $Np+1$ conditions of the system (49) are linearly independent. So there exist k-step IE^{N-1}-LMMs of order k.
II. The order of accuracy of a k-step IE^{N-1}-LMM is at most k.
III. The family of k-step IE^{N-1}-LMM of order k has k free parameters.

Similar to the argument in section 4, one can generalize the following corollary.

Corollary 2. *Any k-step IE^{N-1}-LMM ($N \ge 3$) of order k reduces to an IMEX-LMM.*

Proof. We use induction. The statement holds for $N = 3$ by Corollary 1. Next, we assume that the statement holds for some $N-2$. Now, an IE^{N-1}-LMM is equivalent to an IE^{N-2}E-LMM, which by assumption reduces to an IEE-LMM, and consequently by Corollary 1, it reduces to an IMEX-LMM. □

8. Conclusions

In this paper, new 3-additive linear multi-step methods are introduced based on two different approaches: two implicit and one explicit discretizations (IIE-LMMs) and one implicit and two explicit discretizations (IEE-LMMs). We systematically derive 3-additive splitting methods up to fourth order and verify their convergence order. A stability analysis is performed on a prototype scalar linear DRA equation, showing the new methods give satisfactory stability results and in some cases are A- or A_0-stable. In addition, the stability regions of the new 3-additive methods are compared with some popular IMEX methods, and it is shown that the new methods have larger stability regions in some cases. Results on maximal attainable order for a given number of steps are provided, along with corresponding generalizations to N-additive splitting methods. In particular, we show that the class of k-step, order-k (N-additive) IE^{N-1}-LMMs reduce to the class of (2-additive) IMEX methods. The performance of the 3-additive methods is tested by comparing them with some popular IMEX methods on a stiff variation of the standard Brusselator problem. The experiments show 3-additive splitting methods can outperform comparable IMEX methods through the combination of improved stability, improved computational expense per step, and no significant degradation in accuracy.

Acknowledgements

Raed Ali Mara'Beh, and the rest of the authors of the UGR, acknowledges the support of grant PID2020-117846GB-I00 from the Spanish government and the María de Maeztu Excellence Unit IMAG, reference CEX2020-001105-M, funded by MCIN/AEI/10.13039/501100011033/, also P. González and Raed MaraBeh acknowledges the support of the Andalusian-Spanish Research Group FQM191. Raymond J. Spiteri acknowledges support from the National Sciences and Engineering Research Council of Canada (NSERC) under Discovery Grant RGPN-2020-04467.

Appendix A. Order conditions

Table A.5
IIE-LMMs order conditions.

k	Order Conditions	
$k=1$	$\begin{aligned} 1+a_0 &= 0, \\ 1 &= b_{-1}^{[1]}+b_0^{[1]}, \\ 1 &= b_{-1}^{[2]}+b_0^{[2]}, \\ 1 &= b_0^{[3]}. \end{aligned}$	IIE1 order conditions
$k=2$	$\begin{aligned} 1+a_0+a_1 &= 0, \\ 1-a_1 &= b_{-1}^{[1]}+b_0^{[1]}+b_1^{[1]}, \\ 1-a_1 &= b_{-1}^{[2]}+b_0^{[2]}+b_1^{[2]}, \\ 1-a_1 &= b_0^{[3]}+b_1^{[3]}, \\ 1+a_1 &= 2b_{-1}^{[1]}-2b_1^{[1]}, \\ 1+a_1 &= 2b_{-1}^{[2]}-2b_1^{[2]}, \\ 1+a_1 &= -2b_1^{[3]}. \end{aligned}$	IIE2 order conditions
$k=3$	$\begin{aligned} 1+a_0+a_1+a_2 &= 0, \\ 1-a_1-2a_2 &= b_{-1}^{[1]}+b_0^{[1]}+b_1^{[1]}+b_2^{[1]}, \\ 1-a_1-2a_2 &= b_{-1}^{[2]}+b_0^{[2]}+b_1^{[2]}+b_2^{[2]}, \\ 1-a_1-2a_2 &= b_0^{[3]}+b_1^{[3]}+b_2^{[3]}, \\ 1+a_1+4a_2 &= 2b_{-1}^{[1]}-2b_1^{[1]}-4b_2^{[1]}, \\ 1+a_1+4a_2 &= 2b_{-1}^{[2]}-2b_1^{[2]}-4b_2^{[2]}, \\ 1+a_1+4a_2 &= -2b_1^{[3]}-4b_2^{[3]}, \\ 1-a_1-8a_2 &= 3b_{-1}^{[1]}+3b_1^{[1]}+12b_2^{[1]}, \\ 1-a_1-8a_2 &= 3b_{-1}^{[2]}+3b_1^{[2]}+12b_2^{[2]}, \\ 1-a_1-8a_2 &= 3b_1^{[3]}+12b_2^{[3]}. \end{aligned}$	IIE3 order conditions
$k=4$	$\begin{aligned} 1+a_0+a_1+a_2+a_3 &= 0, \\ 1-a_1-2a_2-3a_3 &= b_{-1}^{[1]}+b_0^{[1]}+b_1^{[1]}+b_2^{[1]}+b_3^{[1]}, \\ 1-a_1-2a_2-3a_3 &= b_{-1}^{[2]}+b_0^{[2]}+b_1^{[2]}+b_2^{[2]}+b_3^{[2]}, \\ 1-a_1-2a_2-3a_3 &= b_0^{[3]}+b_1^{[3]}+b_2^{[3]}+b_3^{[3]}, \\ 1+a_1+4a_2+9a_3 &= 2b_{-1}^{[1]}-2b_1^{[1]}-4b_2^{[1]}-6b_3^{[1]}, \\ 1+a_1+4a_2+9a_3 &= 2b_{-1}^{[2]}-2b_1^{[2]}-4b_2^{[2]}-6b_3^{[2]}, \\ 1+a_1+4a_2+9a_3 &= -2b_1^{[3]}-4b_2^{[3]}-6b_3^{[3]}, \\ 1-a_1-8a_2-27a_3 &= 3b_{-1}^{[1]}+3b_1^{[1]}+12b_2^{[1]}+27b_3^{[1]}, \\ 1-a_1-8a_2-27a_3 &= 3b_{-1}^{[2]}+3b_1^{[2]}+12b_2^{[2]}+27b_3^{[2]}, \\ 1-a_1-8a_2-27a_3 &= 3b_1^{[3]}+12b_2^{[3]}+27b_3^{[3]}, \\ 1+a_1+16a_2+81a_3 &= 4b_{-1}^{[1]}-4b_1^{[1]}-32b_2^{[1]}-108b_3^{[1]}, \\ 1+a_1+16a_2+81a_3 &= 4b_{-1}^{[2]}-4b_1^{[2]}-32b_2^{[2]}-108b_3^{[2]}, \\ 1+a_1+16a_2+81a_3 &= -4b_1^{[3]}-32b_2^{[3]}-108b_3^{[3]}. \end{aligned}$	IIE4 order conditions

Table A.6
IEE-LMMs order conditions.

k	Order Conditions	
$k=2$	$1+a_0+a_1 = 0,$	IEE2 order conditions
	$1-a_1 = b_{-1}^{[1]}+b_0^{[1]}+b_1^{[1]},$	
	$1-a_1 = b_0^{[2]}+b_1^{[2]},$	
	$1-a_1 = b_0^{[3]}+b_1^{[3]}.$	
$k=3$	$1+a_0+a_1+a_2 = 0,$	IEE3 order conditions
	$1-a_1-2a_2 = b_{-1}^{[1]}+b_0^{[1]}+b_1^{[1]}+b_2^{[1]},$	
	$1-a_1-2a_2 = b_0^{[2]}+b_1^{[2]}+b_2^{[2]},$	
	$1-a_1-2a_2 = b_0^{[3]}+b_1^{[3]}+b_2^{[3]},$	
	$1+a_1+4a_2 = 2b_{-1}^{[1]}-2b_1^{[1]}-4b_2^{[1]},$	
	$1+a_1+4a_2 = -2b_1^{[2]}-4b_2^{[2]},$	
	$1+a_1+4a_2 = -2b_1^{[3]}-4b_2^{[3]}.$	
$k=4$	$1+a_0+a_1+a_2+a_3 = 0,$	IEE4 order conditions
	$1-a_1-2a_2-3a_3 = b_{-1}^{[1]}+b_0^{[1]}+b_1^{[1]}+b_2^{[1]}+b_3^{[1]},$	
	$1-a_1-2a_2-3a_3 = b_0^{[2]}+b_1^{[2]}+b_2^{[2]}+b_3^{[2]},$	
	$1-a_1-2a_2-3a_3 = b_0^{[3]}+b_1^{[3]}+b_2^{[3]}+b_3^{[3]},$	
	$1+a_1+4a_2+9a_3 = 2b_{-1}^{[1]}-2b_1^{[1]}-4b_2^{[1]}-6b_3^{[1]},$	
	$1+a_1+4a_2+9a_3 = -2b_1^{[2]}-4b_2^{[2]}-6b_3^{[2]},$	
	$1+a_1+4a_2+9a_3 = -2b_1^{[3]}-4b_2^{[3]}-6b_3^{[3]},$	
	$1-a_1-8a_2-27a_3 = 3b_{-1}^{[1]}+3b_1^{[1]}+12b_2^{[1]}+27b_3^{[1]},$	
	$1-a_1-8a_2-27a_3 = 3b_1^{[2]}+12b_2^{[2]}+27b_3^{[2]},$	
	$1-a_1-8a_2-27a_3 = 3b_1^{[3]}+12b_2^{[3]}+27b_3^{[3]}.$	

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