

ON A NEW CLASS OF BDF AND IMEX SCHEMES FOR PARABOLIC TYPE EQUATIONS

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ABSTRACT. When applying the classical multistep schemes for solving differential equations, one often faces the dilemma that smaller time steps are needed with higher-order schemes, making it impractical to use high-order schemes for stiff problems. We construct in this paper a new class of BDF and implicit-explicit (IMEX) schemes for parabolic type equations based on the Taylor expansions at time $t^{n+\beta}$ with $\beta > 1$ being a tunable parameter. These new schemes, with a suitable β , allow larger time steps at higher-order for stiff problems than that is allowed with a usual higher-order scheme. For parabolic type equations, we identify an explicit uniform multiplier for the new second- to fourth-order schemes, and conduct rigorously stability and error analysis by using the energy argument. We also present ample numerical examples to validate our findings.

1. INTRODUCTION

We consider in this paper numerical methods of a class of nonlinear ordinary or partial differential equations in the form

$$\begin{aligned} u_t + \mathcal{L}u(t) + \mathcal{G}[u(t)] &= f(t), \quad 0 < t < T, \\ u(0) &= u^0, \end{aligned} \tag{1.1}$$

where \mathcal{L} is a linear (or possibly nonlinear) positive operator and \mathcal{G} is a nonlinear operator, whose exact descriptions can be found in the next section.

Numerical approximation of ordinary differential equations (ODEs) is a very mature field (see, for instance, [9, 10, 15, 18]), and the numerical methods developed for ODEs have been playing important roles in solving partial differential equations (PDEs) in the form of (1.1) through the method of lines [27], or the so called method of lines transpose [20], i.e., discretizing first in time followed by the discretization in space. In particular, the backward difference formulae (BDF) and the implicit-explicit (IMEX) schemes are frequently used to deal with (1.1) which exhibit stiff behaviors [8, 16, 21].

Two key issues of numerical methods for (1.1) are stability and accuracy. In order to obtain highly accurate solution with less computational costs, it is highly desirable to be able to use higher-order schemes with larger time steps. However, as we increase the order of accuracy of BDF or IMEX type schemes, their stability regions usually decrease, i.e., smaller time steps need to be used with higher-order schemes, particularly for stiff problems, making high-order schemes impractical for many complex nonlinear systems. A natural question arises: is it possible to develop higher-order multi-step schemes such that their stability regions are comparable or even larger than lower-order classical BDF or IMEX schemes?

The main purposes of this paper are two-fold:

- to construct a new class of BDF and IMEX schemes with a tunable parameter such that larger time steps can be used in higher-order schemes;

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- to carry out a rigorous stability and error analysis for this new class of IMEX schemes.

Furthermore, we provide convincing numerical evidences to validate our theoretical findings.

We recall that the classical BDF and IMEX schemes for approximating solution at time t^{n+1} are usually constructed using the Taylor expansion formulae at time $t^{n+\beta}$ with $\beta \in \{0, 1\}$. In this paper, we shall construct a new class of BDF and IMEX schemes based on the Taylor expansion formulae at time $t^{n+\beta}$ with $\beta \geq 1$ being a tunable parameter. The new schemes are a simple generalization of the classical BDF or IMEX schemes with essentially the same computational efforts. However, they enjoy a remarkable property that their stability regions increase as the parameter β increases, making it possible, by choosing a suitably large β , to use high-order schemes with reasonably larger time steps. The price to pay with a larger β is increased truncation errors which can be more than compensated with higher-order of accuracy.

On the other hand, it is well known that a rigorous stability and error analysis by using the energy technique of the classical BDF (and the related IMEX) schemes of order up to five (cf. [5, 6, 14, 22, 24]) relies on a result by Nevanlinna and Odeh [25] (see also [3] for the extension to the six-order BDF scheme) in which the existence of suitable multiplier that can lead to energy stability was established. It is therefore natural to ask whether such a multiplier exists for the new class of BDF schemes. We shall construct explicitly suitable multipliers in a more general form for the new class of BDF schemes of orders two to four, and derive explicit telescoping formulae associated with these multipliers. Furthermore, for nonlinear parabolic type equations, we show rigorously that the stability condition of the new class of IMEX schemes becomes less restrictive as β increases, particularly compared with the classical case of $\beta = 1$.

The idea behind the new class of BDF and IMEX schemes is very simple but original, and can be easily extended to other type numerical schemes. However, our stability and error analysis rely on the explicit formulae for the uniform multipliers and telescoping decomposition whose derivations are totally nontrivial and original. On the other hand, the new schemes can be easily implemented with a minimal effort by modifying the code based on the classical BDF or IMEX schemes, and provide a much needed improvement on the stability of higher-order schemes.

The rest of the paper is organized as follows. In Section 2, we describe the abstract setting and construct the new class of BDF and IMEX methods based on the Taylor expansion at time $t^{n+\beta}$ and investigate their stability regions. In Section 3, we identify an explicit and uniform multiplier for the new class of BDF and IMEX schemes, which plays an essential role in the stability and error analysis. In Section 4, we establish the unconditional stability for the linear parabolic equations and the stability, followed by error analysis for the nonlinear parabolic equations in Section 5. In section 6, we discuss extension to the fifth-order scheme. In section 7, we provide numerical examples to show the advantages of our new schemes, followed by some concluding remarks in section 8.

2. A NEW CLASS OF BDF AND IMEX SCHEMES

2.1. The abstract setting. We first describe the functional setting. For the sake of simplicity, we consider a simpler setting than that used in [6], although our analysis would also work for the more general setting there.

Let V and H be two real Hilbert spaces such that $V \subset H = H' \subset V'$, with V densely and continuously embedded in H and V' being the dual space of V . We consider (1.1) with $\mathcal{L}: V \rightarrow V'$ being a positive definite, self-adjoint, linear operator, and f in V' is a given source term. We denote the inner product in H by (\cdot, \cdot) , and the induced norm in H by $|\cdot|$. We also denote the norm in V by $\|\cdot\|$ which is defined as $\|u\| := |\mathcal{L}^{1/2}u| = (\mathcal{L}u, u)^{1/2}$. The dual norm in V' is defined by

$$\|v\|_* := \sup_{u \in V \setminus \{0\}} \frac{|(v, u)|}{\|u\|}, \quad \forall v \in V'. \quad (2.1)$$

We assume that the nonlinear operator \mathcal{G} satisfies the following local Lipschitz condition [6] in a ball $\mathcal{B}_{u(t)} := \{v \in V : \|v - u(t)\| \leq 1\}$, centered at the exact solution $u(t)$,

$$\|\mathcal{G}(v) - \mathcal{G}(\tilde{v})\|_*^2 \leq \gamma \|v - \tilde{v}\|^2 + \mu |v - \tilde{v}|^2, \quad \forall v, \tilde{v} \in \mathcal{B}_{u(t)}, \quad \forall t \in [0, T], \quad (2.2)$$

with a non-negative constant γ and an arbitrary constant μ .

2.2. Construction of the new schemes. We shall first construct the new schemes for (1.1) based on the Taylor expansion at time $t^{n+\beta}$. Given an integer $k \geq 2$, denoting $t^n = n\Delta t$, it follows from the Taylor expansion at time $t^{n+\beta}$ that

$$\phi(t^{n+1-i}) = \sum_{m=0}^{k-1} [(1-i-\beta)\Delta t]^m \frac{\phi^{(m)}(t^{n+\beta})}{m!} + \mathcal{O}(\Delta t^k), \quad \text{for } k \geq i \geq 0. \quad (2.3)$$

Then we can derive from the above an implicit difference formula to approximate $\partial_t \phi(t^{n+\beta})$:

$$\frac{1}{\Delta t} \sum_{q=0}^k a_{k,q}(\beta) \phi(t^{n+1-k+q}) = \partial_t \phi(t^{n+\beta}) + \mathcal{O}(\Delta t^k), \quad (2.4)$$

where $a_{k,q}(\beta)$ can be uniquely determined by solving the following linear system with a Vandermonde matrix:

$$\begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ \beta - 1 & \beta & \dots & \dots & \beta + k - 1 \\ (\beta - 1)^2 & \beta^2 & \dots & \dots & (\beta + k - 1)^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (\beta - 1)^k & \beta^k & \dots & \dots & (\beta + k - 1)^k \end{bmatrix} \begin{bmatrix} a_{k,k}(\beta) \\ a_{k,k-1}(\beta) \\ a_{k,k-2}(\beta) \\ \vdots \\ a_{k,0}(\beta) \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \quad (2.5)$$

Similarly, we can derive an implicit difference formula to approximate $\phi(t^{n+\beta})$:

$$\sum_{q=0}^{k-1} b_{k,q}(\beta) \phi(t^{n+2-k+q}) = \phi(t^{n+\beta}) + \mathcal{O}(\Delta t^k), \quad (2.6)$$

with $b_{k,q}(\beta)$ being the unique solution of the following Vandermonde system:

$$\begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ \beta - 1 & \beta & \dots & \dots & \beta + k - 2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (\beta - 1)^{k-1} & \beta^{k-1} & \dots & \dots & (\beta + k - 2)^{k-1} \end{bmatrix} \begin{bmatrix} b_{k,k-1}(\beta) \\ b_{k,k-2}(\beta) \\ \vdots \\ b_{k,0}(\beta) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \quad (2.7)$$

To deal with the nonlinear term in (1.1), we also need the following explicit difference formula to approximate $\phi(t^{n+\beta})$:

$$\sum_{q=0}^{k-1} c_{k,q}(\beta) \phi(t^{n+1-k+q}) = \phi(t^{n+\beta}) + \mathcal{O}(\Delta t^k), \quad (2.8)$$

where $c_{k,q}(\beta)$ can be uniquely determined from:

$$\begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ \beta & \beta + 1 & \dots & \dots & \beta + k - 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \beta^{k-1} & (\beta + 1)^{k-1} & \dots & \dots & (\beta + k - 1)^{k-1} \end{bmatrix} \begin{bmatrix} c_{k,k-1}(\beta) \\ c_{k,k-2}(\beta) \\ \vdots \\ c_{k,0}(\beta) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \quad (2.9)$$

Then, a new class of BDF schemes for (1.1) with $\mathcal{G} = 0$ is

$$\frac{1}{\Delta t} \sum_{q=0}^k a_{k,q}(\beta) \phi^{n+1-k+q} + \mathcal{L} \left(\sum_{q=0}^{k-1} b_{k,q}(\beta) \phi^{n+2-k+q} \right) = f(t^{n+\beta}), \quad k \geq 2, \quad (2.10)$$

and a new class of IMEX schemes for (1.1) is

$$\frac{1}{\Delta t} \sum_{q=0}^k a_{k,q}(\beta) \phi^{n+1-k+q} + \mathcal{L} \left(\sum_{q=0}^{k-1} b_{k,q}(\beta) \phi^{n+2-k+q} \right) + \mathcal{G} \left(\sum_{q=0}^{k-1} c_{k,q}(\beta) \phi^{n+1-k+q} \right) = f(t^{n+\beta}), \quad k \geq 2. \quad (2.11)$$

Remark 1. When $\beta = 1$, (2.11) (resp. (2.10)) becomes the classical semi-implicit IMEX (resp. BDF) schemes, and there have been extensive works regarding its stability and error analysis [2, 4, 6, 22, 23] in the literature. For $\forall \beta > 1$, (2.10) and (2.11) still involve values at the same $k + 1$ -levels as the classical one (with $\beta = 1$) on the left hand side while they involve values at time $t^{n+\beta}$ on the right hand side.

For the reader's convenience, we list below the coefficients in (2.11) for $k = 2, 3, 4$.

$k = 2$:

$$a_{2,2}(\beta) = \frac{2\beta + 1}{2}, \quad a_{2,1}(\beta) = -2\beta, \quad a_{2,0}(\beta) = \frac{2\beta - 1}{2}, \quad (2.12a)$$

$$b_{2,1}(\beta) = \beta, \quad b_{2,0}(\beta) = -(\beta - 1), \quad (2.12b)$$

$$c_{2,1}(\beta) = \beta + 1, \quad c_{2,0}(\beta) = -\beta. \quad (2.12c)$$

$k = 3$:

$$a_{3,3}(\beta) = \frac{3\beta^2 + 6\beta + 2}{6}, \quad a_{3,2}(\beta) = \frac{-(9\beta^2 + 12\beta - 3)}{6}, \quad a_{3,1}(\beta) = \frac{9\beta^2 + 6\beta - 6}{6}, \quad a_{3,0}(\beta) = \frac{-(3\beta^2 - 1)}{6}, \quad (2.13a)$$

$$b_{3,2}(\beta) = \frac{\beta^2 + \beta}{2}, \quad b_{3,1}(\beta) = -(\beta^2 - 1), \quad b_{3,0}(\beta) = \frac{\beta^2 - \beta}{2}, \quad (2.13b)$$

$$c_{3,2}(\beta) = \frac{\beta^2 + 3\beta + 2}{2}, \quad c_{3,1}(\beta) = -(\beta^2 + 2\beta), \quad c_{3,0}(\beta) = \frac{\beta^2 + \beta}{2}. \quad (2.13c)$$

$k = 4$:

$$a_{4,4}(\beta) = \frac{2\beta^3 + 9\beta^2 + 11\beta + 3}{12}, \quad a_{4,3}(\beta) = \frac{-8\beta^3 - 30\beta^2 - 20\beta + 10}{12}, \quad a_{4,2}(\beta) = \frac{12\beta^3 + 36\beta^2 + 6\beta - 18}{12} \\ a_{4,1}(\beta) = \frac{-8\beta^3 - 18\beta^2 + 4\beta + 6}{12}, \quad a_{4,0}(\beta) = \frac{2\beta^3 + 3\beta^2 - \beta - 1}{12}, \quad (2.14a)$$

$$b_{4,3}(\beta) = \frac{\beta^3 + 3\beta^2 + 2\beta}{6}, \quad b_{4,2}(\beta) = \frac{-\beta^3 - 2\beta^2 + \beta + 2}{2}, \quad b_{4,1}(\beta) = \frac{\beta^3 + \beta^2 - 2\beta}{2}, \quad b_{4,0}(\beta) = \frac{-\beta^3 + \beta}{6}, \quad (2.14b)$$

$$c_{4,3}(\beta) = \frac{\beta^3 + 6\beta^2 + 11\beta + 6}{6}, \quad c_{4,2}(\beta) = \frac{-\beta^3 - 5\beta^2 - 6\beta}{2}, \quad c_{4,1}(\beta) = \frac{\beta^3 + 4\beta^2 + 3\beta}{2}, \\ c_{4,0}(\beta) = \frac{-\beta^3 - 3\beta^2 - 2\beta}{6}. \quad (2.14c)$$

Remark 2. Instead of deriving (2.11) from Taylor expansions, one may also derive it by following the standard construction of the usual multistep methods using interpolation formulae (see, e.g., Section 2 in [19]). In fact, it can be shown that the coefficients $a_{k,q}(\beta)$, $b_{k,q}(\beta)$, $c_{k,q}(\beta)$ can be determined by the values at $t^{n+\beta}$ of the corresponding Lagrange polynomials and their derivatives. For example,

$$a_{k,q}(\beta) = \Delta t L'_q(t^{n+\beta}), \quad q = 0, \dots, k, \quad (2.15)$$

where L_q is the Lagrange polynomials associated with $t^{n+1-k}, \dots, t^{n+1}$.

2.3. Linear stability regions. In this subsection, we investigate the regions of linear stability of the new schemes (2.10). For the test equation $\phi_t = \lambda \phi$, (2.10) reduces to

$$\frac{1}{\Delta t} \sum_{q=0}^k a_{k,q}(\beta) \phi^{n+1-k+q} = \lambda \sum_{q=0}^{k-1} b_{k,q}(\beta) \phi^{n+2-k+q}, \quad k \geq 2. \quad (2.16)$$

In order to study the stability regions for $\beta \neq 1$, we set $\phi^n = w^n$ (here, “ n ” is an upper index in ϕ^n and an exponent in w^n) and $z = \lambda\Delta t$ in (2.16) to obtain its characteristic equation, e.g., in the case of $k = 2$, it takes the form:

$$(2\beta + 1 - 2\beta z)w^2 + (2(\beta - 1)z - 4\beta)w + (2\beta - 1) = 0. \quad (2.17)$$

Then the region of absolute stability of method (2.16) is the set of all $z \in \mathbb{C}$ such that the characteristic polynomial satisfies the root condition. We recall that the second order case was already considered in [17], and it was shown that the second-order case of (2.16) is A-stable for $\beta \geq 1$, and more importantly, the stability regions increase as we increase β .

In Fig. 1 and Fig. 2, we plot the stability regions of the general third- and fourth-order BDF schemes for $\beta = 1, 3, 5$. We observe that, the stability regions increase as we increase β .

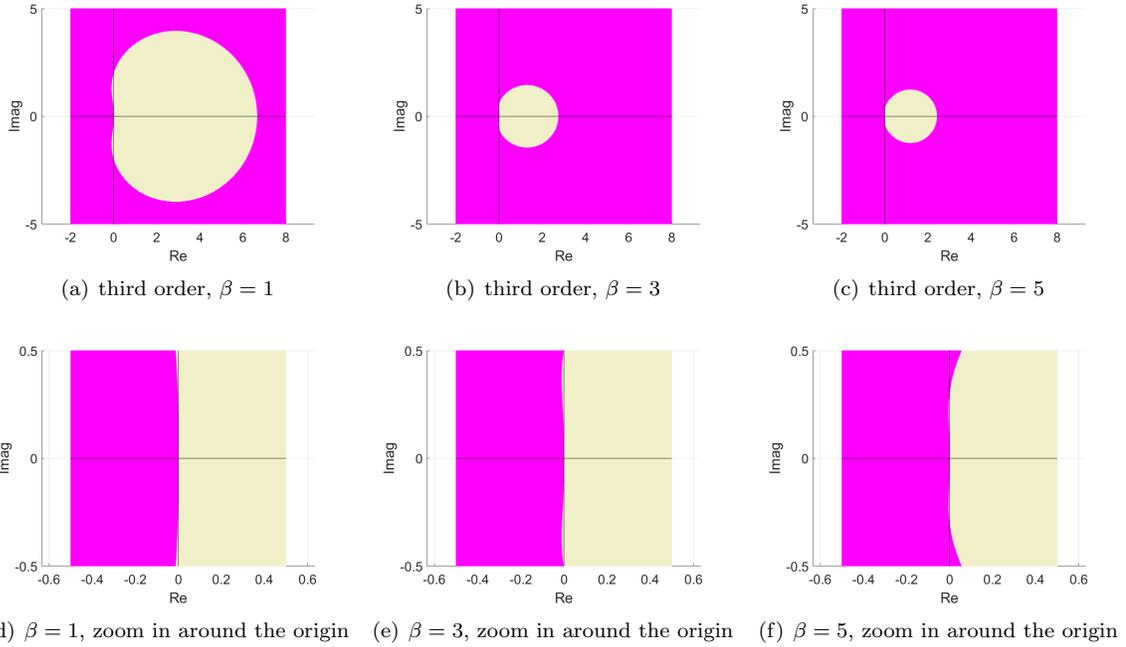


FIGURE 1. The pink parts show the region of absolute stability of the general third order BDF scheme with Taylor expansion at $n + \beta$, $\beta = 1, 3, 5$.

In order to have a better sense on how the stability regions vary with different β and k , we plot in Table 1 a comparison of stability regions in the same scale. We observe that (i) the stability regions increase faster when β is closer to 1; and (ii) the area of the stability region with $k = 4$ and $\beta = 3$ is already bigger than that of the classical second-order BDF. Hence, we can expect that the general fourth-order scheme with $\beta = 3$ allows similar or larger time steps for nonlinear problems than the classical second-order IMEX, avoiding the usual scenario that smaller time step has to be used when increasing the accuracy order.

3. MULTIPLIERS FOR THE NEW BDF AND IMEX SCHEMES

In order to conduct the stability and error analysis for the BDF and IMEX schemes by using energy techniques, a key step is to find a suitable multiplier. A key result which allows one to prove energy stability of the classical BDF schemes of order up to five is established in [25] where the existence of such multiplier is shown, see [3] for extension of this result to six-order BDF. In this section, we

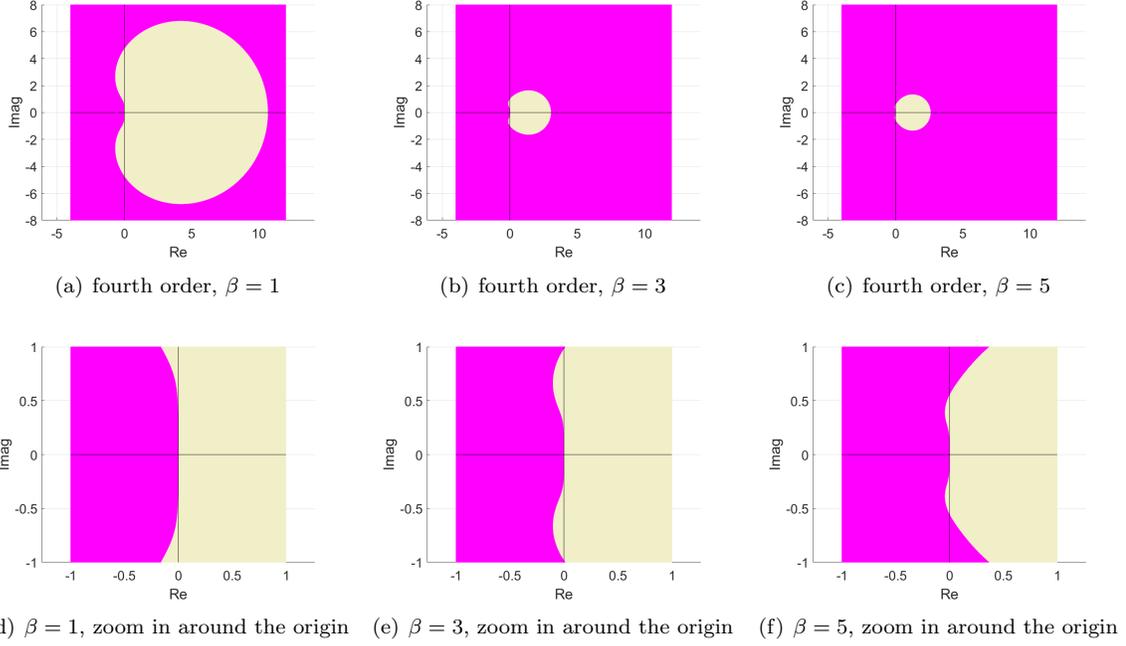


FIGURE 2. The pink parts show the region of absolute stability of the general fourth-order BDF scheme with Taylor expansion at $n + \beta$, $\beta = 1, 3, 5$.

identify an explicit multiplier, and show that it is suitable for the new BDF and IMEX schemes of second to fourth order.

3.1. Notations and a key lemma. To simplify the presentations, we introduce the following notations:

$$A_k^\beta(\phi^i) = \sum_{q=0}^k a_{k,q}(\beta) \phi^{i-k+q}, \quad B_k^\beta(\phi^i) = \sum_{q=0}^{k-1} b_{k,q}(\beta) \phi^{i-k+1+q}, \quad C_k^\beta(\phi^i) = \sum_{q=0}^{k-1} c_{k,q}(\beta) \phi^{i-k+1+q}. \quad (3.1)$$

with $a_{k,q}$, $b_{k,q}$, $c_{k,q}$ defined in (2.12), (2.13) and (2.14). We also consider the characteristic polynomials of the new BDF and IMEX schemes (2.10) and (2.11):

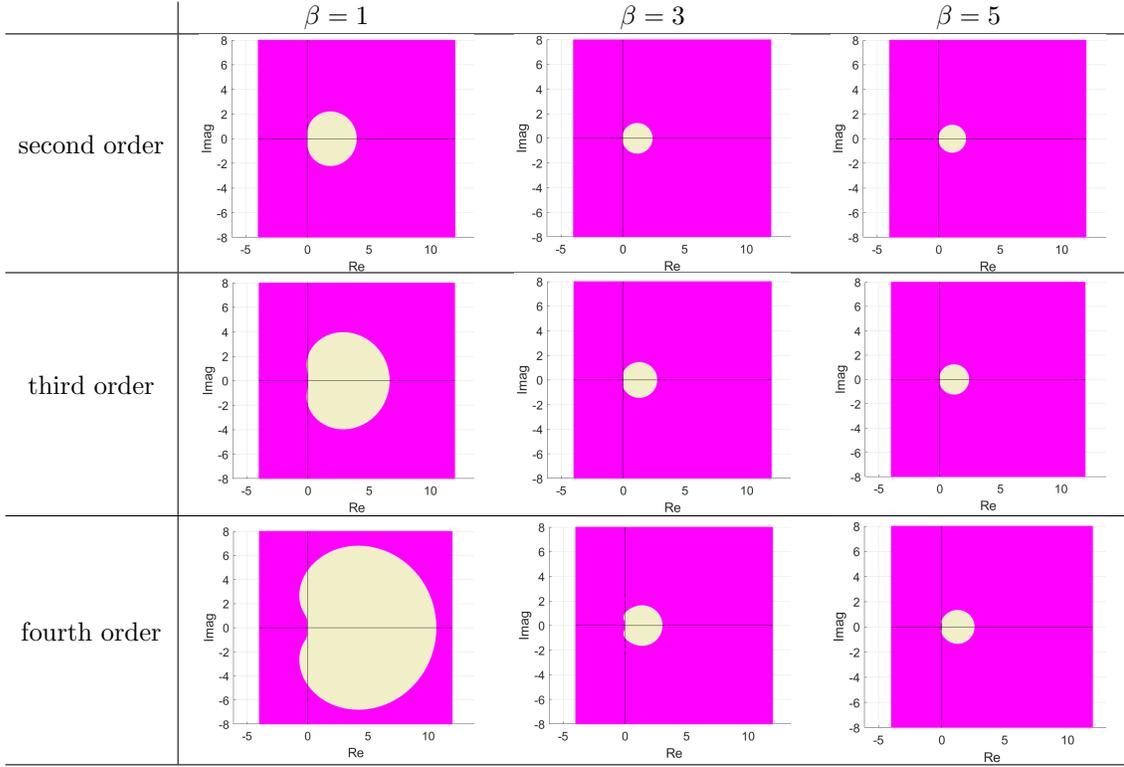
$$\tilde{A}_k^\beta(\zeta) = \sum_{q=0}^k a_{k,q}(\beta) \zeta^q, \quad k = 2, 3, 4; \quad (3.2a)$$

$$\tilde{C}_k^\beta(\zeta) = \sum_{q=0}^{k-1} c_{k,q}(\beta) \zeta^q, \quad k = 2, 3, 4. \quad (3.2b)$$

We first recall the following result from Dahlquist's G-stability theory [13] which plays a key role in establishing energy stability of multistep methods.

Lemma 1. *Let $\alpha(\zeta) = \alpha_k \zeta^k + \dots + \alpha_0$ and $\mu(\zeta) = \mu_k \zeta^k + \dots + \mu_0$ be polynomials of degree at most k (and at least one of them of degree k) that have no common divisors. Let (\cdot, \cdot) be an inner product with associated norm $|\cdot|$. If*

$$\operatorname{Re} \frac{\alpha(\zeta)}{\mu(\zeta)} > 0 \quad \text{for } |\zeta| > 1, \quad (3.3)$$

TABLE 1. Comparison of stability regions for different k and β on the same scale.

then there exists a symmetric positive definite matrix $G = (g_{ij}) \in \mathbb{R}^{k \times k}$ and real $\delta_0, \dots, \delta_k$ such that for v^0, \dots, v^k in the inner product space,

$$\left(\sum_{i=0}^k \alpha_i v^i, \sum_{j=0}^k \mu_j v^j \right) = \sum_{i,j=1}^k g_{ij} (v^i, v^j) - \sum_{i,j=1}^k g_{ij} (v^{i-1}, v^{j-1}) + \left| \sum_{i=0}^k \delta_i v^i \right|^2. \quad (3.4)$$

It is clear from the above Lemma that the key for establishing the energy stability of (2.11) is to find a suitable multiplier $\mu(\zeta) = \mu_k \zeta^k + \dots + \mu_0$ such that (3.3) is satisfied with $\alpha(\zeta) = \tilde{A}_k^\beta(\zeta)$. To this end, we first split $B_k^\beta(\phi^{n+1})$ into two parts:

$$B_k^\beta(\phi^{n+1}) = \eta_k(\beta) C_k^\beta(\phi^{n+1}) + D_k^\beta(\phi^{n+1}), \quad k = 2, 3, 4, \quad (3.5)$$

with

$$\eta_2(\beta) = \frac{\beta-1}{\beta}, \quad \eta_3(\beta) = \frac{\beta-1}{\beta+1}, \quad \eta_4(\beta) = \frac{\beta-1}{\beta+3}, \quad \beta \geq 1, \quad (3.6)$$

and D_k^β can be written as

$$D_k^\beta(\phi^{n+1}) = \sum_{q=0}^{k-1} d_{k,q}(\beta) \phi^{n+2-k+q}, \quad k = 2, 3, 4, \quad (3.7)$$

with

$$d_{2,1}(\beta) = \frac{1}{\beta}, \quad d_{2,0}(\beta) = 0, \quad (3.8a)$$

$$d_{3,2}(\beta) = 1, \quad d_{3,1}(\beta) = \frac{1-\beta}{1+\beta}, \quad d_{3,0}(\beta) = 0, \quad (3.8b)$$

$$d_{4,3}(\beta) = \frac{\beta^2}{6} + \frac{\beta}{2} + \frac{1}{3}, \quad d_{4,2}(\beta) = -\left(\frac{\beta^2}{2} + \frac{\beta}{2} - 1\right), \quad d_{4,1}(\beta) = \frac{\beta(\beta-1)}{2}, \quad d_{4,0}(\beta) = -\frac{\beta(\beta^2-1)}{6(\beta+3)}. \quad (3.8c)$$

We also define

$$\tilde{D}_k^\beta(\zeta) = \sum_{q=0}^{k-1} d_{k,q}(\beta)\zeta^q, \quad k = 2, 3, 4. \quad (3.9)$$

Remark 3. The choices of $\eta_i(\beta)$ are not unique. We choose $\eta_2(\beta), \eta_3(\beta)$ defined in (3.6) to make D_2^β, D_3^β as simple as possible and the choice of $\eta_4(\beta)$ defined in (3.6) allows us to prove (3.13) in the next subsection.

3.2. A uniform multiplier. Note that in [25], it was shown that there exists a multiplier in the form of $\phi^{n+1} - \tilde{\eta}_k \phi^n$ with $\tilde{\eta}_k \geq 0$ for the usual BDF schemes of order 2 to 5. Surprisingly, we can find a uniform multiplier for the new BDF and IMEX schemes of order 2 to 4. More precisely, we have the following results.

Theorem 1. *Given $\beta \geq 1$, then*

$$\gcd(\tilde{A}_k^\beta(\zeta), \zeta \tilde{C}_k^\beta(\zeta)) = \gcd(\tilde{D}_k^\beta(\zeta), \tilde{C}_k^\beta(\zeta)) = 1, \quad k = 2, 3, 4, \quad (3.10)$$

i.e. they have no common divisor, and

$$\operatorname{Re} \frac{\tilde{A}_k^\beta(\zeta)}{\zeta \tilde{C}_k^\beta(\zeta)} > 0, \quad \text{for } |\zeta| > 1, \quad k = 2, 3, 4. \quad (3.11)$$

Moreover, we also have

$$\operatorname{Re} \frac{\tilde{D}_k^\beta(\zeta)}{\tilde{C}_k^\beta(\zeta)} > 0, \quad \text{for } |\zeta| > 1, \quad k = 2, 3; \quad (3.12)$$

and finally if $\beta \geq 2$, then we also have

$$\operatorname{Re} \frac{\tilde{D}_4^\beta(\zeta)}{\tilde{C}_4^\beta(\zeta)} > 0, \quad \text{for } |\zeta| > 1. \quad (3.13)$$

Proof. The proof follows the basic process in [3]. We will provide the proof for the case $k = 4$ in detail as it includes some technical estimations and then we will point out the key steps for the cases $k = 2, 3$, which are easier to handle. To simplify the notation, we often omit the dependence on β for the coefficients $a_{k,q}(\beta), c_{k,q}(\beta), d_{k,q}(\beta)$, i.e., we only write them as $a_{k,q}, c_{k,q}, d_{k,q}$.

Case I: $k = 4$. Firstly, we show $\gcd(\tilde{A}_4^\beta(\zeta), \zeta \tilde{C}_4^\beta(\zeta)) = 1$ by using the **Sylvester Resultant** [1] as follows. The Sylvester matrix [1] of $\tilde{A}_4^\beta(\zeta)$ and $\tilde{C}_4^\beta(\zeta)$ is

$$\operatorname{Sly}(\tilde{A}_4^\beta, \tilde{C}_4^\beta) = \begin{pmatrix} a_{4,4} & a_{4,3} & a_{4,2} & a_{4,1} & a_{4,0} & 0 & 0 \\ 0 & a_{4,4} & a_{4,3} & a_{4,2} & a_{4,1} & a_{4,0} & 0 \\ 0 & 0 & a_{4,4} & a_{4,3} & a_{4,2} & a_{4,1} & a_{4,0} \\ c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} & 0 & 0 & 0 \\ 0 & c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} & 0 & 0 \\ 0 & 0 & c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} & 0 \\ 0 & 0 & 0 & c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} \end{pmatrix}. \quad (3.14)$$

It is easy to verify that its determinant is

$$\det \text{Sl}y(\tilde{A}_4^\beta, \tilde{C}_4^\beta) = -\frac{1}{5184}(18\beta^6 + 144\beta^5 + 426\beta^4 + 566\beta^3 + 321\beta^2 + 55\beta + 3) \neq 0, \quad \text{for } \beta \geq 1, \quad (3.15)$$

which implies that $\gcd(\tilde{A}_4^\beta(\zeta), \tilde{C}_4^\beta(\zeta)) = 1$. Combined with $\tilde{A}_4^\beta(0) = a_{4,0} \neq 0$, it also implies that $\tilde{A}_4^\beta(\zeta)$ and $\zeta\tilde{C}_4^\beta(\zeta)$ have no common divisor.

Next, we show $\frac{\tilde{A}_4^\beta(\zeta)}{\zeta\tilde{C}_4^\beta(\zeta)}$ is holomorphic outside the unit disk in the complex plane. To this end, it suffices to show that all three zeros of $\tilde{C}_4^\beta(\zeta)$ are inside the unit disk. Note that

$$\frac{d\tilde{C}_4^\beta}{dx}(x) = 3c_{4,3}x^2 + 2c_{4,2}x + c_{4,1}, \quad (3.16)$$

with

$$c_{4,3} = \frac{\beta^3 + 6\beta^2 + 11\beta + 6}{6} > 0, \quad \Delta_4 := 4c_{4,2}^2 - 12c_{4,3}c_{4,1} = -\beta(\beta + 2)(\beta + 3)^2 < 0, \quad (3.17)$$

which means $\tilde{C}_4^\beta(x)$ is monotonically increasing in the real axis. Note also that

$$\tilde{C}_4^\beta(0) = c_{4,0} = -\frac{\beta^3 + 3\beta^2 + 2\beta}{6} < 0, \quad \tilde{C}_4^\beta(1) = c_{4,3} + c_{4,2} + c_{4,1} + c_{4,0} = 1. \quad (3.18)$$

Therefore, $\tilde{C}_4^\beta(\zeta) = 0$ has exactly one real root, denoted as x_1 , and two complex roots, denoted as $z_2, z_3 = \bar{z}_2$, in the complex plane. Next, we denote

$$x_0 := \frac{-c_{4,0}}{c_{4,3} - 1} = \frac{\beta^2 + 3\beta + 2}{\beta^2 + 6\beta + 11}. \quad (3.19)$$

Then we can find with $\beta \geq 1$,

$$\tilde{C}_4^\beta(x_0) = -\frac{2\beta^6 + 27\beta^5 + 141\beta^4 + 351\beta^3 + 405\beta^2 + 162\beta - 8}{(\beta^2 + 6\beta + 11)^3} < 0. \quad (3.20)$$

Combining (3.18) and (3.20), we have $x_0 < x_1 < 1$. On the other hand, by Vieta's formulae, we have

$$x_1 z_2 z_3 = x_1 |z_2|^2 = -\frac{c_{4,0}}{c_{4,3}}, \quad \text{then } |z_2|^2 = \frac{1 - c_{4,0}}{x_1 c_{4,3}} < \frac{1 - c_{4,0}}{x_0 c_{4,3}} = \frac{c_{4,3} - 1}{c_{4,3}} < 1. \quad (3.21)$$

As a result, we have $|x_1|, |z_2|, |z_3| < 1$ and hence $\frac{\tilde{A}_4^\beta(\zeta)}{\zeta\tilde{C}_4^\beta(\zeta)}$ and $\frac{\tilde{D}_4^\beta(\zeta)}{\tilde{C}_4^\beta(\zeta)}$ are holomorphic outside the unit disk.

On the other hand, we have

$$\lim_{|\zeta| \rightarrow \infty} \frac{\tilde{A}_4^\beta(\zeta)}{\zeta\tilde{C}_4^\beta(\zeta)} = \frac{a_{4,4}}{c_{4,3}} = \frac{2\beta^3 + 9\beta^2 + 11\beta + 3}{2(\beta^3 + 6\beta^2 + 11\beta + 6)} > 0. \quad (3.22)$$

Therefore, it follows from the maximum principle for harmonic functions, $\text{Re} \frac{\tilde{A}_4^\beta(\zeta)}{\zeta\tilde{C}_4^\beta(\zeta)} > 0, \forall |\zeta| > 1$ is equivalent to

$$\text{Re} \frac{\tilde{A}_4^\beta(\zeta)}{\zeta\tilde{C}_4^\beta(\zeta)} \geq 0, \quad \forall \zeta \in \mathbb{S}^1, \quad (3.23)$$

with \mathbb{S}^1 being the unit circle in the complex plane, and which is equivalent to

$$\text{Re}[\tilde{A}_4^\beta(e^{i\theta})e^{-i\theta}\tilde{C}_4^\beta(e^{-i\theta})] \geq 0, \quad \theta \in [0, 2\pi). \quad (3.24)$$

Letting $y := \cos(\theta)$ and using the trigonometric identities

$$\cos(2\theta) = 2y^2 - 1, \quad \cos(3\theta) = 4y^3 - 3y, \quad \sin(2\theta) = 2y\sin(\theta), \quad \sin(3\theta) = (4y^2 - 1)\sin(\theta), \quad (3.25)$$

we find

$$\begin{aligned}\tilde{C}_4^\beta(e^{-i\theta}) &= c_{4,3} \cos(3\theta) + c_{4,2} \cos(2\theta) + c_{4,1} \cos(\theta) + c_{4,0} - i[c_{4,3} \sin(3\theta) + c_{4,2} \sin(2\theta) + c_{4,1} \sin(\theta)] \\ &= c_{4,3}(4y^3 - 3y) + c_{4,2}(2y^2 - 1) + c_{4,1}y + c_{4,0} - i[c_{4,3}(4y^2 - 1) + 2c_{4,2}y + c_{4,1}] \sin(\theta),\end{aligned}\quad (3.26)$$

and

$$\begin{aligned}\tilde{A}_4^\beta(e^{i\theta})e^{-i\theta} &= a_{4,4}e^{3i\theta} + a_{4,3}e^{2i\theta} + a_{4,2}e^{i\theta} + a_{4,1} + a_{4,0}e^{-i\theta} \\ &= a_{4,4} \cos(3\theta) + a_{4,3} \cos(2\theta) + a_{4,2} \cos(\theta) + a_{4,1} + a_{4,0} \cos(\theta) \\ &\quad + i[a_{4,4} \sin(3\theta) + a_{4,3} \sin(2\theta) + a_{4,2} \sin(\theta) - a_{4,0} \sin(\theta)] \\ &= a_{4,4}(4y^3 - 3y) + a_{4,3}(2y^2 - 1) + (a_{4,2} + a_{4,0})y + a_{4,1} \\ &\quad + i[a_{4,4}(4y^2 - 1) + 2a_{4,3}y + a_{4,2} - a_{4,0}] \sin(\theta).\end{aligned}\quad (3.27)$$

It follows from (3.26), (3.27) and $\tilde{A}_4^\beta(1) = 0$, $\sin^2(\theta) = 1 - y^2$ that

$$\operatorname{Re}[\tilde{A}_4^\beta(e^{i\theta})e^{-i\theta}\tilde{C}_4^\beta(e^{-i\theta})] = \frac{1}{9}(1-y)(\omega_3(\beta)y^3 + \omega_2(\beta)y^2 + \omega_1(\beta)y + \omega_0(\beta)) =: \frac{1}{9}(1-y)f_4(y), \quad (3.28)$$

with

$$\begin{aligned}f_4(y) &= \omega_3(\beta)y^3 + \omega_2(\beta)y^2 + \omega_1(\beta)y + \omega_0(\beta), \\ \omega_0(\beta) &= 2\beta^6 + 15\beta^5 + 39\beta^4 + 39\beta^3 + 10\beta^2 + 15, \\ \omega_1(\beta) &= -6\beta^6 - 45\beta^5 - 117\beta^4 - 116\beta^3 - 21\beta^2 + 17\beta + 9, \\ \omega_2(\beta) &= 6\beta^6 + 45\beta^5 + 117\beta^4 + 115\beta^3 + 12\beta^2 - 34\beta - 12, \\ \omega_3(\beta) &= -2\beta^6 - 15\beta^5 - 39\beta^4 - 38\beta^3 - \beta^2 + 17\beta + 6.\end{aligned}\quad (3.29)$$

In the following, we omit the dependence on β for ω_i , $i = 0, 1, 2, 3$.

It is clear that (3.24) is equivalent to

$$f_4(y) \geq 0, \quad \forall y \in [-1, 1]. \quad (3.30)$$

With ω_i defined in (3.29) and $\beta \geq 1$, we have

$$\begin{aligned}f_4(1) &= \omega_0 + \omega_1 + \omega_2 + \omega_3 = 18 > 0, \\ f_4(-1) &= \omega_0 - \omega_1 + \omega_2 - \omega_3 = 16\beta^6 + 120\beta^5 + 312\beta^4 + 308\beta^3 + 44\beta^2 - 68\beta - 12 > 0,\end{aligned}\quad (3.31)$$

and

$$f_4'(y) = 3\omega_3y^2 + 2\omega_2y + \omega_1. \quad (3.32)$$

If $f_4'(y)$ does not have zero in $[-1, 1]$, then (3.31) implies (3.30). Otherwise, supposing there exists $-1 \leq y_0 \leq 1$ such that $f_4'(y_0) = 0$, we only need to show $f_4(y_0) \geq 0$. Indeed, with $f_4'(y_0) = 0$, we have

$$3f_4(y_0) = 3f_4(y_0) - y_0f_4'(y_0) = \omega_2y_0^2 + 2\omega_1y_0 + 3\omega_0. \quad (3.33)$$

Denote

$$g_4(y) := \omega_2y^2 + 2\omega_1y + 3\omega_0; \quad (3.34)$$

then with $\beta \geq 1$, we have

$$\begin{aligned}g_4(1) &= \omega_2 + 2\omega_1 + 3\omega_0 = 51 > 0, \\ g_4(-1) &= \omega_2 - 2\omega_1 + 3\omega_0 = 24\beta^6 + 180\beta^5 + 468\beta^4 + 464\beta^3 + 84\beta^2 - 68\beta + 15 > 0, \\ \Delta_g &= 4\omega_1^2 - 12\omega_2\omega_0 = -1220\beta^6 - 9108\beta^5 - 23408\beta^4 - 22212\beta^3 - 1076\beta^2 + 7344\beta + 2484 < 0,\end{aligned}\quad (3.35)$$

which means $g_4(y) > 0, \forall y \in [-1, 1]$. In particular, we have $f_4(y_0) = \frac{1}{3}g_4(y_0) > 0$ which implies (3.30), which in turn implies (3.24). Therefore, we proved (3.11) with $k = 4$.

Next, we prove (3.13) with $\beta \geq 2$. The procedure is similar to the proof of (3.11) above. First, the Sylvester matrix of $\tilde{D}_4^\beta(\zeta)$ and $\tilde{C}_4^\beta(\zeta)$:

$$\text{Sly}(\tilde{D}_4^\beta, \tilde{C}_4^\beta) = \begin{pmatrix} d_{4,3} & d_{4,2} & d_{4,1} & d_{4,0} & 0 & 0 \\ 0 & d_{4,3} & d_{4,2} & d_{4,1} & d_{4,0} & 0 \\ 0 & 0 & d_{4,3} & d_{4,2} & d_{4,1} & d_{4,0} \\ c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} & 0 & 0 \\ 0 & c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} & 0 \\ 0 & 0 & c_{4,3} & c_{4,2} & c_{4,1} & c_{4,0} \end{pmatrix}, \quad (3.36)$$

and its determinant is

$$\det \text{Sly}(\tilde{D}_4^\beta, \tilde{C}_4^\beta) = -\frac{\beta^2(\beta^2 + 3\beta + 2)^2}{36} < 0 \quad (3.37)$$

which implies $\tilde{D}_4^\beta(\zeta)$ and $\tilde{C}_4^\beta(\zeta)$ have no common divisor. Since we have shown in the above that $\frac{\tilde{D}_4^\beta(\zeta)}{\tilde{C}_4^\beta(\zeta)}$ is holomorphic outside the unit disk, following the same process as above, we have that (3.13) is equivalent to:

$$h_4(y) = \alpha_3(\beta)y^3 + \alpha_2(\beta)y^2 + \alpha_1(\beta)y + \alpha_0(\beta) \geq 0, \quad \forall y \in [-1, 1], \quad (3.38)$$

with

$$\begin{aligned} \alpha_0(\beta) &= \frac{1}{9(\beta+3)}(2\beta^6 + 15\beta^5 + 35\beta^4 + 15\beta^3 - 37\beta^2 - 39\beta + 9), \\ \alpha_1(\beta) &= -\frac{2\beta^5}{3} - 3\beta^4 - \frac{10\beta^3}{3} + \beta^2 + 2\beta + 1, \\ \alpha_2(\beta) &= \frac{1}{3}(\beta(2\beta^4 + 9\beta^3 + 12\beta^2 + 3\beta - 2)), \\ \alpha_3(\beta) &= -\frac{1}{9}(\beta(\beta+1)^2(2\beta^2 + 5\beta + 2)). \end{aligned} \quad (3.39)$$

In the following, we omit the dependence on β for $\alpha_i, i = 0, 1, 2, 3$. Hence, we have

$$\begin{aligned} h_4(-1) &= -\alpha_3 + \alpha_2 - \alpha_1 + \alpha_0 = \frac{2}{9(\beta+3)}(8\beta^6 + 60\beta^5 + 152\beta^4 + 132\beta^3 - 16\beta^2 - 57\beta - 9) > 0, \\ h_4(1) &= \alpha_3 + \alpha_2 + \alpha_1 + \alpha_0 = \frac{4}{\beta+3} > 0, \end{aligned} \quad (3.40)$$

and

$$h'_4(y) = 3\alpha_3y^2 + 2\alpha_2y + \alpha_1. \quad (3.41)$$

Similarly as before, if $h'_4(y)$ does not have zero in $[-1, 1]$, then (3.40) implies (3.38). Suppose $-1 \leq y_0 \leq 1$ such that $h'_4(y_0) = 0$, we only need to show $h_4(y_0) \geq 0$.

With $h'_4(y_0) = 0$ and $\alpha_3 \neq 0$, we have

$$\begin{aligned} 3h_4(y_0) &= 3h_4(y_0) - y_0h'_4(y_0) = \alpha_2y_0^2 + 2\alpha_1y_0 + 3\alpha_0 \\ &= \frac{\alpha_2}{3\alpha_3}h'_4(y_0) + (2\alpha_1 - \frac{2\alpha_2^2}{3\alpha_3})y_0 + 3\alpha_0 - \frac{\alpha_1\alpha_2}{3\alpha_3} \\ &= 0 + (2\alpha_1 - \frac{2\alpha_2^2}{3\alpha_3})y_0 + 3\alpha_0 - \frac{\alpha_1\alpha_2}{3\alpha_3}. \end{aligned} \quad (3.42)$$

We define

$$p(y) := (2\alpha_1 - \frac{2\alpha_2^2}{3\alpha_3})y + 3\alpha_0 - \frac{\alpha_1\alpha_2}{3\alpha_3}. \quad (3.43)$$

Then $p(y^*) = 0$ if we define y^* as

$$y^* := \frac{\frac{\alpha_1\alpha_2}{3\alpha_3} - 3\alpha_0}{2\alpha_1 - \frac{2\alpha_2^2}{3\alpha_3}} = \frac{4\beta^4 + 30\beta^3 + 35\beta^2 + 3\beta}{4\beta^4 + 30\beta^3 + 71\beta^2 + 54\beta + 9}, \quad (3.44)$$

and we also have

$$2\alpha_1 - \frac{2\alpha_2^2}{3\alpha_3} = \frac{8\beta^2 + 28\beta + 6}{6\beta + 3} > 0. \quad (3.45)$$

Therefore, to prove (3.38), it suffices to show $y_0 \geq y^*$. However, this is more complicated as (3.44) implies that y^* can be arbitrarily close to 1 by increasing β , and meanwhile, there indeed exists $y^* < y_0 < 1$ such that $h'_4(y_0) = 0$.

It follows from (3.41) that

$$y_0 = \frac{-2\alpha_2 \pm \sqrt{\Delta_h}}{6\alpha_3}, \quad (3.46)$$

with

$$\Delta_h := 4\alpha_2^2 - 12\alpha_1\alpha_3 = \frac{4\beta(\beta+1)^2(4\beta^3 + 22\beta^2 + 31\beta + 6)}{9} > 0. \quad (3.47)$$

We can estimate Δ_h as follows

$$\Delta_h < \Delta_h + \frac{4(\beta+1)^2(2\beta^3 + 5\beta^2 - 6\beta)}{9} = \frac{4}{9}(\beta+1)^2(2\beta^2 + 6\beta)^2 =: \Delta_h^*. \quad (3.48)$$

To show $y_0 \geq y^*$, we only consider the smallest root of $h'_4(y) = 0$. Since we have $\alpha_2 > 0$ and $\alpha_3 < 0$, the smallest root is

$$y_0 = \frac{-2\alpha_2 + \sqrt{\Delta_h}}{6\alpha_3} > \frac{-2\alpha_2 + \sqrt{\Delta_h^*}}{6\alpha_3} = \frac{2\beta^3 + 7\beta^2 + 3\beta - 8}{2\beta^3 + 7\beta^2 + 7\beta + 2}. \quad (3.49)$$

Finally, we can prove $y_0 \geq y^*$ as follows. It follows from (3.44) and (3.49) that

$$\begin{aligned} y_0 - y^* &> \frac{2\beta^3 + 7\beta^2 + 3\beta - 8}{2\beta^3 + 7\beta^2 + 7\beta + 2} - \frac{4\beta^4 + 30\beta^3 + 35\beta^2 + 3\beta}{4\beta^4 + 30\beta^3 + 71\beta^2 + 54\beta + 9} \\ &= \frac{56\beta^4 + 138\beta^3 - 95\beta^2 - 339\beta - 72}{8\beta^6 + 80\beta^5 + 300\beta^4 + 523\beta^3 + 430\beta^2 + 153\beta + 18}, \end{aligned} \quad (3.50)$$

and given $\beta \geq 2$,

$$\begin{aligned} 56\beta^4 + 138\beta^3 - 95\beta^2 - 339\beta - 72 &\geq 56 \times 2^3\beta + 138 \times 2\beta^2 - 95\beta^2 - 339\beta - 72 \\ &= 109\beta + 181\beta^2 - 72 > 0. \end{aligned} \quad (3.51)$$

Therefore, we have $y_0 \geq y^*$. Hence (3.13) is proved for $\beta \geq 2$.

For the case $k = 2$ and 3, we can prove (3.11) and (3.12) by the same process as above, so we only point out some related facts below, which are sufficient to complete the proof.

Case II: $k = 2$.

- $\det Sly(\tilde{A}_2^\beta, \tilde{C}_2^\beta) = -\frac{1}{2} \neq 0$, $\det Sly(\tilde{D}_2^\beta, \tilde{C}_2^\beta) = -1 \neq 0$, $\tilde{A}_2^\beta(0) \neq 0$.
- The only zero of $\tilde{C}_2^\beta(\zeta)$ is $\frac{\beta}{1+\beta} < 1$, which means $\frac{\tilde{A}_2^\beta(\zeta)}{\zeta\tilde{C}_2^\beta(\zeta)}$ and $\frac{\tilde{D}_2^\beta(\zeta)}{\tilde{C}_2^\beta(\zeta)}$ are holomorphic outside the unit disk.
- For $k = 2$, (3.11) is equivalent to

$$f_2(y) = (-2\beta^2 - \beta + 1)y + 2\beta^2 + \beta + 1 \geq 0, \quad \forall y \in [-1, 1], \quad (3.52)$$

which is true since $f_2(y)$ is monotonically decreasing and $f_2(1) = 2$.

- For $k = 2$, (3.12) is equivalent to

$$h_3(y) = -y + 1 + \frac{1}{\beta} \geq 0, \quad \forall y \in [-1, 1], \quad (3.53)$$

which is obviously true.

Case III: $k = 3$.

- $\det Sly(\tilde{A}_3^\beta, \tilde{C}_3^\beta) = \frac{\beta^2}{8} + \frac{5\beta}{24} + \frac{1}{36} \neq 0$, $\det Sly(\tilde{D}_3^\beta, \tilde{C}_3^\beta) = \frac{\beta(\beta+1)}{2} \neq 0$, $\tilde{A}_3^\beta(0) \neq 0$, $\forall \beta \geq 1$.
- $\tilde{C}_3^\beta(\zeta)$ has two complex zeros z_1 and z_2 such that $|z_1|^2 = |z_2|^2 = \frac{\beta}{\beta+2} < 1$, which means $\frac{\tilde{A}_3^\beta(\zeta)}{\zeta\tilde{C}_3^\beta(\zeta)}$ and $\frac{\tilde{D}_3^\beta(\zeta)}{\tilde{C}_3^\beta(\zeta)}$ are holomorphic outside the unit disk.

- For $k = 3$, (3.11) is equivalent to

$$f_3(y) = \sigma_2(\beta)y^2 + \sigma_1(\beta)y + \sigma_0 \geq 0, \quad \forall y \in [-1, 1], \quad (3.54)$$

with

$$\sigma_2(\beta) = 3\beta^4 + 9\beta^3 + 5\beta^2 - 3\beta - 2, \quad (3.55a)$$

$$\sigma_1(\beta) = -6\beta^4 - 18\beta^3 - 13\beta^2 + \beta + 4, \quad (3.55b)$$

$$\sigma_0(\beta) = 3\beta^4 + 9\beta^3 + 8\beta^2 + 2\beta + 4. \quad (3.55c)$$

(3.54) is true since $\sigma_2(\beta) > 0$ for $\beta \geq 1$ and

$$f_3(-1) = 12\beta^4 + 36\beta^3 + 26\beta^2 - 2\beta - 2 > 0, \quad (3.56a)$$

$$f_3(1) = 6, \quad (3.56b)$$

$$\Delta_3 := \sigma_1^2 - 4\sigma_0\sigma_2 = -63\beta^4 - 186\beta^3 - 95\beta^2 + 72\beta + 48 < 0. \quad (3.56c)$$

- For $k = 3$, (3.12) is equivalent to

$$h_3(y) = \mu_2(\beta)y^2 + \mu_1(\beta)y + \mu_0(\beta) \geq 0, \quad \forall y \in [-1, 1], \quad (3.57)$$

with

$$\mu_2(\beta) = \beta(\beta + 1), \quad (3.58a)$$

$$\mu_1(\beta) = -2\beta^2 - 2\beta + 1, \quad (3.58b)$$

$$\mu_0(\beta) = \frac{\beta^3 + 2\beta^2 + 1}{\beta + 1}. \quad (3.58c)$$

(3.57) is true since $\mu_2(\beta) > 0$ for $\beta \geq 1$ and

$$h_3(-1) = \frac{2\beta(2\beta^2 + 4\beta + 1)}{\beta + 1} > 0, \quad (3.59a)$$

$$h_3(1) = \frac{2}{\beta + 1} > 0, \quad (3.59b)$$

$$\Delta_3^* := \mu_1^2 - 4\mu_0\mu_2 = 1 - 8\beta < 0. \quad (3.59c)$$

The proof for all the cases is completed. \square

Remark 4. The restriction $\beta \geq 2$ is a sufficient condition for (3.13), which comes from (3.51). One can easily show that (3.37) and (3.51) are true whenever $\beta > 1.6$. On the other hand, (3.38) is not true when $\beta = 1$ as $h_4(0.2) = -0.312 < 0$ with h_4 defined in (3.38).

3.3. Explicit telescoping formulae for the second and third order schemes. Note that Lemma 1 only provides the existence of a symmetric positive definite matrix G without giving the exact value of g_{ij} . In the following, we provide explicit formulae for g_{ij} in the second and third order cases.

Proposition 3.1. *For the second-order version of (2.11), we have*

$$(D_2^\beta(\phi^{n+1}), C_2^\beta(\phi^{n+1})) = \frac{1}{\beta}|\phi^{n+1}|^2 + \frac{1}{2}|\phi^{n+1}|^2 - \frac{1}{2}|\phi^n|^2 + \frac{1}{2}|\phi^{n+1} - \phi^n|^2, \quad (3.60)$$

and

$$\begin{aligned} (A_2^\beta(\phi^{n+1}), C_2^\beta(\phi^{n+1})) &= a_2|\phi^{n+1}|^2 - a_2|\phi^n|^2 + |b_2\phi^{n+1} + c_2\phi^n|^2 - |b_2\phi^n + c_2\phi^{n-1}|^2 \\ &\quad + |d_2\phi^{n+1} + e_2\phi^n + f_2\phi^{n-1}|^2, \end{aligned} \quad (3.61)$$

where the coefficients are given by

$$\begin{aligned} e_2 &= -\sqrt{2\beta(2\beta+1)}, \Delta_2 = 2\beta(2\beta+1), c_2 = f_2 = \frac{-\sqrt{2} + \sqrt{\Delta_2}}{2}, \\ d_2 &= \sqrt{2} + f_2, E_2 = -\beta(2\beta-1), b_2 = \frac{E_2 - 2e_2f_2}{-2c}, a_2 = \frac{3\beta+1 - 2\sqrt{\beta(2\beta+1)}}{2(\beta+1)^2}. \end{aligned}$$

Moreover, we have $a_2 > 0$ for all $\beta \geq 1$.

Proposition 3.2. For the third-order version of (2.11), we have

$$\begin{aligned} (D_3^\beta(\phi^{n+1}), C_3^\beta(\phi^{n+1})) &= \hat{a}_3|\phi^{n+1}|^2 - \hat{a}_3|\phi^n|^2 + |\hat{b}_3\phi^{n+1} + \hat{c}_3\phi^n|^2 - |\hat{b}_3\phi^n + \hat{c}_3\phi^{n-1}|^2 \\ &\quad + |\hat{d}_3\phi^{n+1} + \hat{e}_3\phi^n + \hat{f}_3\phi^{n-1}|^2, \end{aligned} \quad (3.62)$$

where the coefficients are given by

$$\begin{aligned} \hat{M} &= \frac{2\beta^3 + 4\beta^2 + \beta + 1}{\beta + 1}, \hat{N} = \frac{(2\beta^2 + 2\beta - 1)^2}{4}, \hat{\Delta}_3 = \hat{M}^2 - 4\hat{N} = \frac{4\beta(2\beta^2 + 4\beta + 1)}{(\beta + 1)^2} \\ \hat{e}_3 &= -\sqrt{\frac{\hat{M} - \sqrt{\hat{\Delta}_3}}{2}}, \hat{P} = \frac{\beta^3 + 2\beta^2 + 1}{\beta + 1} - \hat{e}_3^2, \hat{Q} = \frac{2\beta^3 + 4\beta^2 + \beta + 1}{\beta + 1} - \hat{e}_3^2, \\ \hat{f}_3 &= \frac{-\sqrt{\hat{P}} + \sqrt{\hat{Q}}}{2}, \hat{c}_3 = \hat{f}_3, \hat{d}_3 = \sqrt{\hat{P}} + \hat{f}_3, \hat{b}_3 = \frac{\beta(\beta - 1) + 4\hat{e}_3\hat{f}_3}{4\hat{c}_3}, \hat{a}_3 = \frac{\beta^2}{2} + \frac{3\beta}{2} + 1 - \hat{b}_3^2 - \hat{d}_3^2; \end{aligned} \quad (3.63)$$

and

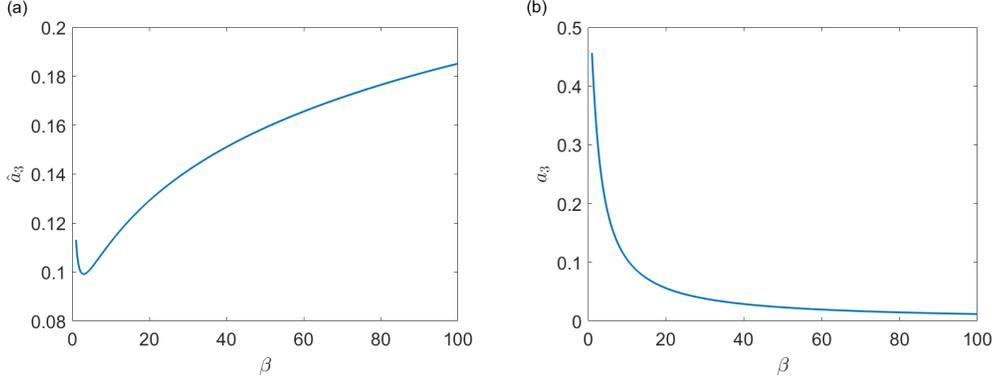
$$\begin{aligned} (A_3^\beta(\phi^{n+1}), C_3^\beta(\phi^{n+1})) &= a_3|\phi^{n+1}|^2 - a_3|\phi^n|^2 + |b_3\phi^{n+1} + c_3\phi^n|^2 - |b_3\phi^n + c_3\phi^{n-1}|^2 \\ &\quad + |d_3\phi^{n+1} + e_3\phi^n + f_3\phi^{n-1}|^2 - |d_3\phi^n + e_3\phi^{n-1} + f_3\phi^{n-2}|^2 + |g_3\phi^{n+1} + h_3\phi^n + i_3\phi^{n-1} + j_3\phi^{n-2}|^2, \end{aligned} \quad (3.64)$$

where the coefficients are given by

$$\begin{aligned} M &= 2\beta^4 + 6\beta^3 + \frac{13\beta^2}{3} - \frac{\beta}{3} - \frac{1}{3}, N = -\left(\frac{\beta^2}{2} - \frac{1}{6}\right)\left(\frac{\beta^2}{2} + \frac{3\beta}{2} + 1\right), P = \frac{\sqrt{M} + 1}{2}, \\ Q &= -\frac{1}{2}\left(\beta\left(\frac{\beta^2}{2} - \frac{1}{6}\right)(\beta + 1)\right), R = \beta^4 + \frac{7\beta^3}{2} + \frac{19\beta^2}{6} - \frac{\beta}{3} - 1, S = \frac{7\beta^4}{4} + \frac{25\beta^3}{4} + \frac{17\beta^2}{3} + \frac{\beta}{2} + \frac{1}{3}, \\ W &= \left(\frac{\beta^2}{2} + \frac{3\beta}{2} + 1\right)\left(\frac{\beta^2}{2} + \beta + \frac{1}{3}\right), U = \frac{1}{2} - \frac{79\beta^2}{12} - \frac{21\beta^3}{4} - \frac{5\beta^4}{4} - \frac{23\beta}{12}, \\ f_3 &= \frac{\sqrt{P^2 + 2N} + P}{2}, j_3 = f_3, g_3 = f_3 - P, i_3 = -\sqrt{M} - g_3, h_3 = \sqrt{M} - f_3, e_3 = \frac{2i_3j_3 - Q}{2f_3}, \\ d_3 &= \frac{R - 2g_3i_3}{2f_3}, c_3 = \sqrt{S - e_3^2 - g_3^2 - h_3^2}, b_3 = \frac{U - 2d_3e_3 - 2g_3h_3}{2c_3}, a_3 = W - g_3^2 - d_3^2 - b_3^2. \end{aligned} \quad (3.65)$$

Moreover, it is numerically verified that all variables appearing in (3.63) and (3.65) are real and bounded, and $\hat{a}_3, a_3 > 0$ for $1 \leq \beta \leq 100$ (cf. Fig. 3).

The proof of the above two propositions is based on the method of undetermined coefficients, more precisely, we assume a desired form and use the method of undetermined coefficients to find the suitable coefficients. The detail of the proof is tedious but straightforward so we leave it to the interested readers.

FIGURE 3. Values of \hat{a}_3 and a_3 with different β .

4. STABILITY OF (2.10) FOR LINEAR PARABOLIC TYPE EQUATIONS

We consider in this section the new BDF schemes for the linear case (2.10), which can be written as

$$\frac{A_k^\beta(\phi^{n+1})}{\Delta t} + \mathcal{L}B_k^\beta(\phi^{n+1}) = f^{n+\beta}, \quad k = 2, 3, 4, \quad (4.1)$$

and establish a stability result based on Theorem 1.

Theorem 2. *Assuming $\|f(t)\|_*^2 \leq C_f, \forall t \leq T, \beta > 1$ for $k = 2, 3$, and $\beta \geq 2$ for $k = 4$, then the scheme (4.1) is stable in the sense that*

$$g_k |\phi^{n+1}|^2 + \frac{1}{2} \Delta t \eta_k(\beta) \sum_{q=k}^{n+1} \|C_k^\beta(\phi^q)\|^2 \leq C \sum_{q=0}^{k-1} (|\phi^q|^2 + \Delta t \|\phi^q\|^2) + \frac{TC_f}{2\eta_k(\beta)}, \quad \forall k \leq n+1 \leq \frac{T}{\Delta t}, \quad (4.2)$$

with g_k a positive constant depending only on k , C a constant independent of Δt and $\eta_k(\beta)$ is defined in (3.6).

Proof. We denote $f^i = f(t^i), \forall i \leq \frac{T}{\Delta t}$. Taking the inner product of (4.1) with $\Delta t C_k^\beta(\phi^{n+1})$ and splitting $B_k^\beta(\phi^{n+1})$ as in (3.5), we obtain

$$(A_k^\beta(\phi^{n+1}), C_k^\beta(\phi^{n+1})) + \Delta t \eta_k(\beta) \|C_k^\beta(\phi^{n+1})\|^2 + \Delta t (\mathcal{L}D_k^\beta(\phi^{n+1}), C_k^\beta(\phi^{n+1})) = \Delta t (f^{n+\beta}, C_k^\beta(\phi^{n+1})), \quad (4.3)$$

where we used $(\mathcal{L}C_k^\beta(\phi^{n+1}), C_k^\beta(\phi^{n+1})) = \|C_k^\beta(\phi^{n+1})\|^2$. We estimate the terms in (4.3) as follows.

It follows from (2.1) and the assumption on f that

$$\begin{aligned} (f^{n+\beta}, C_k^\beta(\phi^{n+1})) &\leq \|f^{n+\beta}\|_* \|C_k^\beta(\phi^{n+1})\| \\ &\leq \frac{1}{2\eta_k(\beta)} \|f^{n+\beta}\|_*^2 + \frac{\eta_k(\beta)}{2} \|C_k^\beta(\phi^{n+1})\|^2 \\ &\leq \frac{C_f}{2\eta_k(\beta)} + \frac{\eta_k(\beta)}{2} \|C_k^\beta(\phi^{n+1})\|^2. \end{aligned} \quad (4.4)$$

Denote $\Phi_k^{n+1} := (\phi^{n-k+1}, \dots, \phi^{n+1})^T$. It follows from Lemma 1 and Theorem 1 that there exist symmetric positive definite matrices $G = (g_{ij}) \in \mathbb{R}^{k \times k}$ and $H = (h_{ij}) \in \mathbb{R}^{(k-1) \times (k-1)}$ such that

$$\begin{aligned} (A_k^\beta(\phi^{n+1}), C_k^\beta(\phi^{n+1})) &\geq \sum_{i,j=1}^k g_{ij} (\phi^{n+1+i-k}, \phi^{n+1+j-k}) - \sum_{i,j=1}^k g_{ij} (\phi^{n+i-k}, \phi^{n+j-k}) \\ &=: |\Phi_k^{n+1}|_G^2 - |\Phi_k^n|_G^2, \end{aligned} \quad (4.5)$$

and

$$\begin{aligned} (\mathcal{L}D_k^\beta(\phi^{n+1}), C_k^\beta(\phi^{n+1})) &\geq \sum_{i,j=1}^{k-1} h_{ij}(\mathcal{L}\phi^{n+2+i-k}, \phi^{n+2+j-k}) - \sum_{i,j=1}^{k-1} h_{ij}(\mathcal{L}\phi^{n+1+i-k}, \phi^{n+1+j-k}) \\ &=: \|\Phi_k^{n+1}\|_H^2 - \|\Phi_k^n\|_H^2. \end{aligned} \quad (4.6)$$

Now, combining (4.3)-(4.6), we obtain

$$|\Phi_k^{n+1}|_G^2 - |\Phi_k^n|_G^2 + \Delta t(\|\Phi_k^{n+1}\|_H^2 - \|\Phi_k^n\|_H^2) + \frac{1}{2}\Delta t\eta_k(\beta)\|C_k^\beta(\phi^{n+1})\|^2 \leq \frac{C_f\Delta t}{2\eta_k(\beta)}. \quad (4.7)$$

Summing up (4.7) from $n = k - 1$ to $n = m$, we obtain

$$|\Phi_k^{m+1}|_G^2 + \Delta t\|\Phi_k^{m+1}\|_H^2 + \frac{1}{2}\Delta t\eta_k(\beta) \sum_{q=k-1}^m \|C_k^\beta(\phi^{q+1})\|^2 \leq |\Phi_k^{k-1}|_G^2 + \Delta t\|\Phi_k^{k-1}\|_H^2 + \frac{TC_f}{2\eta_k(\beta)}. \quad (4.8)$$

Let g_k be the smallest eigenvalue of the matrix $G \in \mathbb{R}^{k,k}$, then we have

$$|\Phi_k^{m+1}|_G^2 \geq g_k|\phi^{m+1}|^2, \quad (4.9)$$

and we can choose a constant C large enough such that

$$|\Phi_k^{k-1}|_G^2 \leq C \sum_{i=0}^{k-1} |\phi^i|^2, \quad (4.10a)$$

$$\Delta t\|\Phi_k^{k-1}\|_H^2 \leq C\Delta t \sum_{i=0}^{k-1} \|\phi^i\|^2. \quad (4.10b)$$

Finally, combining (4.8) and (4.10) leads to

$$g_k|\phi^{m+1}|^2 + \frac{1}{2}\Delta t\eta_k(\beta) \sum_{q=k-1}^m \|C_k^\beta(\phi^{q+1})\|^2 \leq C \sum_{i=0}^{k-1} (|\phi^i|^2 + \Delta t\|\phi^i\|^2) + \frac{TC_f}{2\eta_k(\beta)}, \quad (4.11)$$

which implies (4.2). \square

Remark 5. Note that in order to obtain (4.6), the linear operator \mathcal{L} is required to be self-adjoint while using the Nevanlinna-Odeh approach in [25] can also deal with \mathcal{L} which is not self-adjoint.

5. STABILITY AND ERROR ANALYSIS OF (2.11) FOR NONLINEAR PARABOLIC TYPE EQUATIONS

In this section, we use the stability result established in the last section to carry out a stability and error analysis of (2.11) for nonlinear parabolic equations.

5.1. Stability. Under the local Lipschitz condition (2.2) on the nonlinear operator \mathcal{G} , we can derive a local stability result for (2.11) similarly as in the proof of the linear case (cf. Theorem 2) if we further assume

$$C_k^\beta(\phi^n) \in \mathcal{B}_{\phi(t^{n+\beta})}, \quad (5.1)$$

with $\beta > 1$ for $k = 2, 3$, and $\beta \geq 2$ for $k = 4$. Note that formally (5.1) must be true when Δt small enough since $C_k^\beta(\phi^n)$ is a k -th order approximation to $\phi(t^{n+\beta})$. We shall defer the rigorous proof of (5.1) to subsection 5.3 by induction together with the error analysis.

5.2. Truncation errors. Using the notations introduced in previous sections, we define the truncation errors for $k = 2, 3, 4$ as

$$E_k^{n+1} := \Delta t \phi_t(t^{n+\beta}) - A_k^\beta(\phi(t^{n+1})), \quad (5.2a)$$

$$R_k^{n+1} := \phi(t^{n+\beta}) - B_k^\beta(\phi(t^{n+1})), \quad (5.2b)$$

$$P_k^n := \phi(t^{n+\beta}) - C_k^\beta(\phi(t^n)). \quad (5.2c)$$

It follows from (2.4), (2.6) and (2.8) that

$$E_k^{n+1} = \mathcal{O}(\Delta t^{k+1}), \quad R_k^{n+1} = \mathcal{O}(\Delta t^k), \quad P_k^n = \mathcal{O}(\Delta t^k). \quad (5.3)$$

More precisely, one can verify

$$E_k^{n+1} = \frac{1}{k!} \sum_{q=0}^k a_{k,q}(\beta) \int_{t^{n+1+q-k}}^{t^{n+\beta}} (t^{n+1+q-k} - s)^k \phi^{(k+1)}(s) ds, \quad (5.4a)$$

$$R_k^{n+1} = \frac{1}{(k-1)!} \sum_{q=0}^{k-1} b_{k,q}(\beta) \int_{t^{n+2+q-k}}^{t^{n+\beta}} (t^{n+2+q-k} - s)^{k-1} \phi^{(k)}(s) ds, \quad (5.4b)$$

$$P_k^n = \frac{1}{(k-1)!} \sum_{q=0}^{k-1} c_{k,q}(\beta) \int_{t^{n+1+q-k}}^{t^{n+\beta}} (t^{n+1+q-k} - s)^{k-1} \phi^{(k)}(s) ds. \quad (5.4c)$$

Therefore, under suitable regularity requirements, we have

$$|E_k^{n+1}|^2 \leq C(\Delta t)^{2k+2}, \quad \|R_k^{n+1}\|^2 \leq C(\Delta t)^{2k}, \quad \|P_k^n\|^2 \leq C(\Delta t)^{2k}, \quad \forall n+1 \leq \frac{T}{\Delta t}. \quad (5.5)$$

5.3. Error estimate. We denote $e^m := \phi^m - \phi(t^m)$, where $\phi(t^m)$ is the exact solution of (1.1) at time t^m , i.e.,

$$\phi_t(t^m) + \mathcal{L}\phi(t^m) + \mathcal{G}[\phi(t^m)] = f(t^m). \quad (5.6)$$

We will use the following discrete version of the Gronwall lemma [26].

Lemma 2. *Let y^k, h^k, g^k, f^k be four nonnegative sequences satisfying*

$$y^n + \Delta t \sum_{k=0}^n h^k \leq B + \Delta t \sum_{k=0}^n (g^k y^k + f^k) \quad \text{with} \quad \Delta t \sum_{k=0}^{T/\Delta t} g^k \leq M, \quad \forall 0 \leq n \leq T/\Delta t.$$

We assume $\Delta t g^k < 1$ for all k , and let $\sigma = \max_{0 \leq k \leq T/\Delta t} (1 - \Delta t g^k)^{-1}$. Then

$$y^n + \Delta t \sum_{k=1}^n h^k \leq \exp(\sigma M) (B + \Delta t \sum_{k=0}^n f^k), \quad \forall n \leq T/\Delta t.$$

Theorem 3. *Assume (2.2) and the solution of (1.1) is sufficiently smooth such that (5.5) is true, and the following stability condition*

$$\eta_k(\beta) - \sqrt{\gamma} \geq \rho > 0 \quad (5.7)$$

is satisfied. Given $\phi^0 = \phi(0) \in V$, we assume $\beta > 1$ for $k = 2, 3$, and $\beta \geq 2$ for $k = 4$, and that $\phi^i, i = 1, \dots, k-1$, are computed with a proper initialization procedure such that

$$|\phi^i - \phi(t^i)|^2, \|\phi^i - \phi(t^i)\|^2 \leq C(\Delta t)^{2k}, \quad i = 1, \dots, k-1, \quad \text{and} \quad C_k^\beta(\phi^{k-1}) \in \mathcal{B}_{\phi(t^{k-1+\beta})}; \quad (5.8)$$

then for Δt sufficiently small, we have

$$C_k^\beta(\phi^{n+1}) \in \mathcal{B}_{\phi(t^{n+1+\beta})}, \quad \forall n+1 \leq \frac{T}{\Delta t}, \quad (5.9)$$

and

$$g_k |e^{n+1}|^2 + \frac{\rho}{2} \Delta t \sum_{q=k-1}^{n+1} \|C_k(e^q)\|^2 \leq C \exp((1 - C\Delta t)^{-1}T) (\Delta t)^{2k}, \quad \forall n+1 \leq \frac{T}{\Delta t}, \quad (5.10)$$

where g_k is a positive constant depending only on k , C is a constant independent of Δt .

Proof. We shall prove (5.9) and (5.10) by induction. Suppose we already have

$$C_k^\beta(\phi^n) \in \mathcal{B}_{\phi(t^{n+\beta})}, \quad \forall n \leq m, \quad (5.11)$$

and (5.10) is satisfied with all $n \leq m-1$, we need to prove

$$C_k^\beta(\phi^{m+1}) \in \mathcal{B}_{\phi(t^{m+1+\beta})}, \quad (5.12)$$

and (5.10) is satisfied with all $n \leq m$.

Subtracting (5.6) with $m = n + \beta$ from (2.11) and multiplying by Δt , we obtain

$$A_k^\beta(e^{n+1}) + \Delta t \mathcal{L} B_k^\beta(e^{n+1}) = -\Delta t (\mathcal{G}[C_k^\beta(\phi^n)] - \mathcal{G}[\phi(t^{n+\beta})]) + E_k^{n+1} + \Delta t \mathcal{L} R_k^{n+1} \quad (5.13)$$

where E_k^{n+1} , R_k^{n+1} are given in (5.2). We split $\mathcal{G}[C_k^\beta(\phi^n)] - \mathcal{G}[\phi(t^{n+\beta})]$ as

$$\begin{aligned} \mathcal{G}[C_k^\beta(\phi^n)] - \mathcal{G}[\phi(t^{n+\beta})] &= (\mathcal{G}[C_k^\beta(\phi^n)] - \mathcal{G}[C_k^\beta(\phi(t^n))]) + (\mathcal{G}[C_k^\beta(\phi(t^n))] - \mathcal{G}[\phi(t^{n+\beta})]) \\ &=: T_1^n + T_2^n. \end{aligned} \quad (5.14)$$

Taking the inner product of (5.13) with $C_k^\beta(e^{n+1})$, and splitting $B_k^\beta(e^{n+1})$ as in (3.5), we obtain

$$\begin{aligned} (A_k^\beta(e^{n+1}), C_k^\beta(e^{n+1})) + \Delta t \eta_k(\beta) \|C_k^\beta(e^{n+1})\|^2 + \Delta t (\mathcal{L} D_k^\beta(e^{n+1}), C_k^\beta(e^{n+1})) \\ = -\Delta t (T_1^n, C_k^\beta(e^{n+1})) - \Delta t (T_2^n, C_k^\beta(e^{n+1})) + (E_k^{n+1}, C_k^\beta(e^{n+1})) + \Delta t (\mathcal{L} R_k^{n+1}, C_k^\beta(e^{n+1})). \end{aligned} \quad (5.15)$$

Next, we bound the right hand side of (5.15) with the help of the consistency estimate. First, it follows from (2.8) that with Δt sufficiently small, we have $C_k^\beta(\phi(t^n)) \in \mathcal{B}_{\phi(t^{n+\beta})}$, then for the terms with T_1^n and T_2^n , it follows from (2.2) and (5.11) that for any given $\varepsilon > 0$,

$$|(T_1^n, C_k^\beta(e^{n+1}))| \leq \|T_1^n\|_* \|C_k^\beta(e^{n+1})\| \leq \frac{\varepsilon}{2} (\gamma \|C_k^\beta(e^n)\|^2 + \mu |C_k^\beta(e^n)|^2) + \frac{1}{2\varepsilon} \|C_k^\beta(e^{n+1})\|^2, \quad (5.16)$$

With P_k^n defined in (5.2), we have

$$\begin{aligned} |(T_2^n, C_k^\beta(e^{n+1}))| &\leq \|T_2^n\|_* \|C_k^\beta(e^{n+1})\| \leq \frac{1}{\rho} (\gamma \|P_k^n\|^2 + \mu |P_k^n|^2) + \frac{\rho}{4} \|C_k^\beta(e^{n+1})\|^2, \\ &\leq C(\Delta t)^{2k} + \frac{\rho}{4} \|C_k^\beta(e^{n+1})\|^2. \end{aligned} \quad (5.17)$$

Similarly,

$$(E_k^{n+1}, C_k^\beta(e^{n+1})) \leq \frac{1}{2\Delta t} |E_k^{n+1}|^2 + \frac{\Delta t}{2} |C_k^\beta(e^{n+1})|^2 \leq C(\Delta t)^{2k+1} + \frac{\Delta t}{2} |C_k^\beta(e^{n+1})|^2, \quad (5.18)$$

and

$$(\mathcal{L} R_k^{n+1}, C_k^\beta(e^{n+1})) \leq \frac{1}{\rho} \|R_k^{n+1}\|^2 + \frac{\rho}{4} \|C_k^\beta(e^{n+1})\|^2 \leq C(\Delta t)^{2k} + \frac{\rho}{4} \|C_k^\beta(e^{n+1})\|^2. \quad (5.19)$$

Now, under the stability condition (5.7), combining the assumption on the initial steps (5.8) and estimations in (5.16)-(5.19), taking $\varepsilon = \frac{1}{\sqrt{\gamma}}$ in (5.16), and following the same process as in the proof of Theorem 2 to handle the terms on the left hand side of (5.15), we can obtain the following from (5.15):

$$g_k |e^{n+1}|^2 + \frac{\rho}{2} \Delta t \sum_{q=k-1}^{n+1} \|C_k^\beta(e^q)\|^2 \leq C \Delta t \sum_{q=0}^{n+1} |e^q|^2 + C(\Delta t)^{2k}, \quad \forall n \leq m. \quad (5.20)$$

Therefore, by applying the discrete Gronwall lemma 2 to (5.20), we can obtain

$$g_k |e^{m+1}|^2 + \frac{\rho}{2} \Delta t \sum_{q=k-1}^{m+1} \|C_k^\beta(e^q)\|^2 \leq C \exp((1 - C\Delta t)^{-1} T) (\Delta t)^{2k}, \quad \forall m+1 \leq \frac{T}{\Delta t}, \quad (5.21)$$

with C a constant independent of Δt which implies (5.10). Finally, it follows from (5.21) and (2.8) that

$$\begin{aligned} \|C_k^\beta(\phi^{m+1}) - \phi(t^{m+1+\beta})\|^2 &\leq 2\|C_k^\beta(\phi^{m+1}) - C_k^\beta(\phi(t^{m+1}))\|^2 + 2\|C_k^\beta(\phi(t^{m+1})) - \phi(t^{m+1+\beta})\|^2 \\ &\leq 2\|C_k^\beta(e^{m+1})\|^2 + \mathcal{O}(\Delta t^{2k}) \\ &\leq \bar{C}\Delta t^{2k-1}, \end{aligned} \tag{5.22}$$

with \bar{C} a constant independent of Δt , which implies (5.12) for Δt sufficiently small. Thus, the proof is complete with the induction. \square

Remark 6. Note that $\eta_k(\beta)$ in (3.6) monotonically increases as β increases. On the other hand, for many applications, given $\delta > 0$, one can choose $\gamma < \delta$ with a suitable μ such that (2.2) is satisfied [6]. Hence, the stability condition (5.7) can always be satisfied with these applications.

Remark 7. The analysis in Theorem 2 and Theorem 3 can not be directly extended to the standard BDF methods (with $\beta = 1$) since $\eta_k(1) = 0$.

5.4. Comparison to the classical BDF and IMEX schemes. In this subsection, we compare the stability condition (5.7) to that of the classical BDF and IMEX methods (with Taylor expansion at time t^{n+1}) for which the stability condition (5.7) does not apply. So we shall derive below a corresponding stability condition for the classical BDF and IMEX methods. To simplify the presentation, we assume $\mu = 0$ in (2.2) since the general case can be handled by applying the discrete Gronwall lemma as in Theorem 3.

The stability condition (5.7) in Theorem 3 is derived from

$$(\mathcal{L}B_k^\beta(e^n), C_k^\beta(e^n)) = (\eta_k(\beta)C_k^\beta(e^n) + D_k^\beta(e^n), C_k^\beta(e^n)) = \eta_k(\beta)\|C_k^\beta(e^n)\|^2 + (D_k^\beta(e^n), C_k^\beta(e^n)), \tag{5.23}$$

and

$$\begin{aligned} (\mathcal{G}[C_k^\beta(\phi^n)] - \mathcal{G}[C_k^\beta(\phi(t^n))], C_k^\beta(e^n)) &\leq \min_{\varepsilon > 0} \left(\frac{\varepsilon}{2} \|\mathcal{G}[C_k^\beta(\phi^n)] - \mathcal{G}[C_k^\beta(\phi(t^n))]\|_*^2 + \frac{1}{2\varepsilon} \|C_k^\beta(e^n)\|^2 \right) \\ &\leq \min_{\varepsilon > 0} \left(\frac{\varepsilon\gamma}{2} \|C_k^\beta(e^n)\|^2 + \frac{1}{2\varepsilon} \|C_k^\beta(e^n)\|^2 \right) \\ &\stackrel{\varepsilon = \frac{1}{\sqrt{\gamma}}}{=} \sqrt{\gamma} \|C_k^\beta(e^n)\|^2. \end{aligned} \tag{5.24}$$

As a result, the stability condition (5.7) is derived by requiring $\eta_k(\beta) > \sqrt{\gamma}$ since the term $(D_k^\beta(e^n), C_k^\beta(e^n))$ can be handled by Lemma 1 and Theorem 1.

On the other hand, for the classical IMEX k ($k = 2, 3, 4$) schemes, i.e., (2.11) with $\beta = 1$, the suitable multipliers are given as $e^n - \tilde{\eta}_k e^{n-1}$ [25] and the smallest possible values of $\tilde{\eta}_k$ are

$$\tilde{\eta}_2 = 0, \quad \tilde{\eta}_3 = 0.0836, \quad \tilde{\eta}_4 = 0.2878. \tag{5.25}$$

Hence, the corresponding versions of (5.24) and (5.23) become

$$\begin{aligned}
& \left(\mathcal{G} \left[\sum_{q=0}^{k-1} c_{k,q}(1) \phi^{n-k+1+q} \right] - \mathcal{G} \left[\sum_{q=0}^{k-1} c_{k,q}(1) \phi(t^{n-k+1+q}) \right], e^n - \tilde{\eta}_k e^{n-1} \right) \\
& \leq \min_{\varepsilon > 0} \left(\frac{\varepsilon}{2} \left\| \mathcal{G} \left[\sum_{q=0}^{k-1} c_{k,q}(1) \phi^{n-k+1+q} \right] - \mathcal{G} \left[\sum_{q=0}^{k-1} c_{k,q}(1) \phi(t^{n-k+1+q}) \right] \right\|_*^2 + \frac{1}{2\varepsilon} \|e^n - \tilde{\eta}_k e^{n-1}\|^2 \right) \\
& \leq \min_{\varepsilon > 0} \left(\frac{\varepsilon \gamma}{2} \sum_{q=0}^{k-1} |c_{k,q}(1)| \|e^{n-k+1+q}\|^2 + \frac{1}{2\varepsilon} \|e^n - \tilde{\eta}_k e^{n-1}\|^2 \right) \\
& \leq \min_{\varepsilon > 0} \left(\frac{\varepsilon \gamma}{2} \sum_{q=0}^{k-1} |c_{k,q}(1)| \|e^{n-k+1+q}\|^2 + \frac{1}{2\varepsilon} (\|e^n\|^2 + \tilde{\eta}_k^2 \|e^{n-1}\|^2) \right),
\end{aligned} \tag{5.26}$$

where $c_{k,q}(1)$ are defined in (2.12)-(2.14) with $\beta = 1$, and

$$(\mathcal{L}e^n, e^n - \tilde{\eta}_k e^{n-1}) = \|e^n\|^2 - \tilde{\eta}_k (\mathcal{L}e^n, e^{n-1}) \geq \|e^n\|^2 - \frac{\tilde{\eta}_k}{2} (\|e^n\|^2 + \|e^{n-1}\|^2). \tag{5.27}$$

Combining (5.26) and (5.27), we obtain the following stability condition for the classical IMEX type scheme with multiplier $e^n - \tilde{\eta}_k e^{n-1}$,

$$1 - \tilde{\eta}_k > \min_{\varepsilon > 0} \left(\frac{\varepsilon \gamma}{2} \sum_{q=0}^{k-1} |c_{k,q}(1)| + \frac{1}{2\varepsilon} (1 + \tilde{\eta}_k^2) \right) \geq \sqrt{\tilde{c}_k \gamma (1 + \tilde{\eta}_k^2)}, \tag{5.28}$$

with $\tilde{c}_k = \sum_{q=0}^{k-1} |c_{k,q}(1)|$. Comparing (5.7) with (5.28), we have two remarks:

- From (5.25) and (5.28), we observe that for the classical IMEX schemes, higher-order (i.e., larger k) requires stronger stability condition on the parameter γ appearing in (2.2). It is this requirement on the time step that limits the use of high order scheme in practice.
- On the other hand, for the new class of IMEX schemes, we observe from (3.6) and (5.7) that the stability condition on γ becomes weaker as we increase β . In particular, the new higher-order schemes with a suitable β can be stable with a larger time step than that is allowed with a classical IMEX scheme of the same-order. For example, we have from (3.6) that $\eta_2(2) = \eta_3(3) = \eta_4(5) = 1/2$ which indicates that the stability condition (5.7) of the new fourth-order scheme with $\beta = 5$ and third-order scheme with $\beta = 3$ is the same as that of the second-order classical scheme. Our numerical results in Example 3 below indicate that we can use the maximum allowable time step of the second-order classical scheme in our new third- and fourth-order schemes to obtain more accurate results.

Remark 8. Note that a new multiplier $e^n - \frac{2}{169}e^{n-1} - \frac{11}{169}e^{n-2}$ for the classical BDF3 scheme is reported in [4] and since $\hat{\eta}_3 := \frac{2}{169} + \frac{11}{169} < \tilde{\eta}_3 = 0.0836$, one can obtain milder conditions on γ compared to adopting the Nevanlinna-Odeh multipliers. Nevertheless, we can derive even milder conditions on γ by choosing larger β in our new methods.

6. EXTENSION TO FIFTH-ORDER

In Theorem 1, we found suitable multipliers for the second- and third-order scheme with $\beta \geq 1$ and for the fourth-order scheme with $\beta \geq 2$. In this section, we would like to show numerically that the multiplier we found in section 3 also works for the fifth-order scheme.

Following the same notations as before, we can obtain the coefficients $a_{5,q}(\beta), b_{5,q}(\beta), c_{5,q}(\beta)$ by solving the linear systems (2.5), (2.7) and (2.9) with $k = 5$, respectively. Then we can define $A_5^\beta(\phi^i), B_5^\beta(\phi^i), C_5^\beta(\phi^i)$ as in (3.1). Next, we split $B_5^\beta(\phi^{n+1})$ as

$$B_5^\beta(\phi^{n+1}) = \eta_5(\beta) C_5^\beta(\phi^{n+1}) + D_5^\beta(\phi^{n+1}), \quad \text{with} \quad \eta_5(\beta) = \frac{\beta - 1}{\beta + 15}, \tag{6.1}$$

and define $\tilde{A}_5^\beta(\zeta), \tilde{C}_5^\beta(\zeta), \tilde{D}_5^\beta(\zeta)$ as in (3.2). Following the key steps in the proof of Theorem 1, we present a sequence of numerical results to show that $C_5^\beta(\phi^{n+1})$ is a suitable multiplier for the fifth-order scheme with $6.5 \leq \beta \leq 100$.

- We have $\gcd(\tilde{A}_5^\beta(\zeta), \zeta \tilde{C}_5^\beta(\zeta)) = \gcd(\tilde{D}_5^\beta(\zeta), \tilde{C}_5^\beta(\zeta)) = 1$ since $\tilde{A}_5^\beta(0) = a_{5,0} \neq 0$ and

$$\det \text{Sly}(\tilde{A}_5^\beta, \tilde{C}_5^\beta) = \frac{\beta^{12}}{221184} + \frac{11\beta^{11}}{110592} + \frac{635\beta^{10}}{663552} + \frac{78937\beta^9}{14929920} + \frac{552809\beta^8}{29859840} + \frac{638383\beta^7}{14929920} + \frac{9801769\beta^6}{149299200} + \frac{4912619\beta^5}{74649600} + \frac{765683\beta^4}{18662400} + \frac{225157\beta^3}{15552000} + \frac{6143\beta^2}{2488320} + \frac{2071\beta}{10368000} + \frac{1}{160000} > 0, \quad (6.2)$$

and

$$\det \text{Sly}(\tilde{D}_5^\beta, \tilde{C}_5^\beta) = \frac{\beta^3(\beta^3 + 6\beta^2 + 11\beta + 6)^3}{13824} > 0. \quad (6.3)$$

- Let r_1, r_2, \dots, r_5 be the five roots of $\tilde{C}_5^\beta(\zeta) = 0$, and denote $r_{\max} = \max_{1 \leq i \leq 5} |r_i|$. In Fig. 4, we plot the numerical values of r_{\max} for $0 \leq \beta \leq 100$. We observe that $r_{\max} < 1$ for $0 \leq \beta \leq 100$, which implies $\tilde{C}_5^\beta(\zeta)$ is holomorphic outside the unit disk in the complex plane.

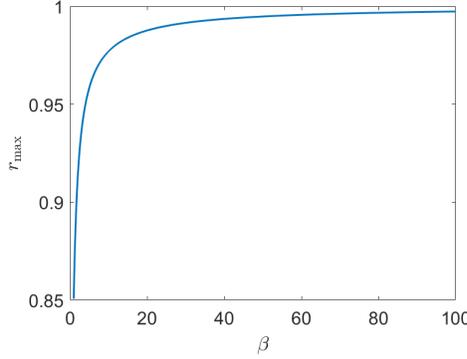


FIGURE 4. r_{\max} with different β .

- Following the same process as in the proof of Theorem 1, we can derive that $\text{Re} \frac{\tilde{A}_5^\beta(\zeta)}{\zeta \tilde{C}_5^\beta(\zeta)} > 0$ for $|\zeta| > 1$ is equivalent to

$$\frac{1}{180}(1-y)f_5(y) \geq 0, \quad \forall y \in [-1, 1],$$

where

$$f_5(y) = \sigma_4(\beta)y^4 + \sigma_3(\beta)y^3 + \sigma_2(\beta)y^2 + \sigma_1(\beta)y + \sigma_0 \geq 0, \quad \forall y \in [-1, 1], \quad (6.4)$$

with

$$\sigma_4(\beta) = 5\beta^8 + 70\beta^7 + 390\beta^6 + 1090\beta^5 + 1539\beta^4 + 820\beta^3 - 350\beta^2 - 540\beta - 144, \quad (6.5a)$$

$$\sigma_3(\beta) = -20\beta^8 - 280\beta^7 - 1550\beta^6 - 4260\beta^5 - 5836\beta^4 - 3024\beta^3 + 950\beta^2 + 1396\beta + 336, \quad (6.5b)$$

$$\sigma_2(\beta) = 30\beta^8 + 420\beta^7 + 2310\beta^6 + 6240\beta^5 + 8244\beta^4 + 3932\beta^3 - 1260\beta^2 - 1340\beta - 204, \quad (6.5c)$$

$$\sigma_1(\beta) = -20\beta^8 - 280\beta^7 - 1530\beta^6 - 4060\beta^5 - 5136\beta^4 - 2072\beta^3 + 1070\beta^2 + 652\beta + 36, \quad (6.5d)$$

$$\sigma_0(\beta) = 5\beta^8 + 70\beta^7 + 380\beta^6 + 990\beta^5 + 1189\beta^4 + 344\beta^3 - 410\beta^2 - 168\beta + 336. \quad (6.5e)$$

- On the other hand, we can also show that $\text{Re} \frac{\tilde{D}_5^\beta(\zeta)}{\tilde{C}_5^\beta(\zeta)} > 0$ for $|\zeta| > 1$ is equivalent to

$$h_5(y) = \mu_4(\beta)y^4 + \mu_3(\beta)y^3 + \mu_2(\beta)y^2 + \mu_1(\beta)y + \mu_0(\beta) \geq 0, \quad \forall y \in [-1, 1], \quad (6.6)$$

with

$$\mu_4(\beta) = \frac{\beta(\beta^2 + 3\beta + 2)^2(6\beta^3 + 37\beta^2 + 48\beta - 27)}{18(\beta + 15)}, \quad (6.7a)$$

$$\mu_3(\beta) = -\frac{\beta(24\beta^7 + 292\beta^6 + 1366\beta^5 + 3013\beta^4 + 2881\beta^3 + 193\beta^2 - 1391\beta - 618)}{18(\beta + 15)}, \quad (6.7b)$$

$$\mu_2(\beta) = \frac{\beta(12\beta^7 + 146\beta^6 + 670\beta^5 + 1385\beta^4 + 1021\beta^3 - 553\beta^2 - 1127\beta - 402)}{6(\beta + 15)}, \quad (6.7c)$$

$$\mu_1(\beta) = -\frac{(24\beta^8 + 292\beta^7 + 1314\beta^6 + 2527\beta^5 + 1203\beta^4 - 2405\beta^3 - 3117\beta^2 - 1008\beta - 270)}{18(\beta + 15)}, \quad (6.7d)$$

$$\mu_0(\beta) = \frac{6\beta^8 + 73\beta^7 + 322\beta^6 + 571\beta^5 + 91\beta^4 - 926\beta^3 - 995\beta^2 - 312\beta + 18}{18(\beta + 15)}. \quad (6.7e)$$

In Fig. 5, we plot the minimum values of $f_5(y)$ and $h_5(y)$ in $[-1, 1]$ with $1 \leq \beta \leq 100$, which show (6.4) is true for $1 \leq \beta \leq 100$ and (6.6) is true for $6.5 \leq \beta \leq 100$. Therefore, we have numerically verified that Theorem 1 is also true for (2.11) with $k = 5$ and $6.5 \leq \beta \leq 100$.

Remark 9. The choice of $\eta_5(\beta)$ in (6.1) is not unique, and the range $6.5 \leq \beta \leq 100$ is not necessarily the largest possible. But our numerical results indicate (6.4) and (6.6) do not hold for some $\beta > 100$.

For the sixth-order scheme, our numerical results show there exists $|r_6| > 1$, which is one root of $\tilde{C}_6^\beta(\zeta) = 0$ and this implies that it is not holomorphic outside the unit disk. Hence, the proof in Theorem 1 can not be extended to the sixth-order.

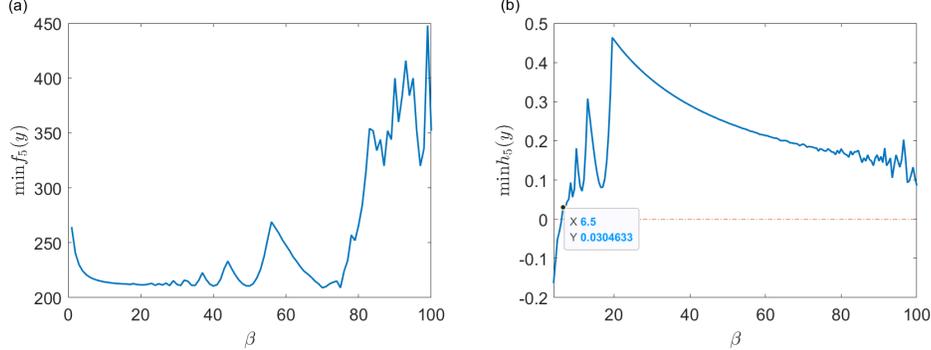


FIGURE 5. Minimum value of f_5 and h_5 in $[-1, 1]$ with different β .

7. NUMERICAL EXAMPLES

In this section, we provide some numerical approximation of the Allen-Cahn [7] and Cahn-Hilliard [11] equations to validate our theoretical results, and to show the advantages of the new IMEX schemes (2.11).

Given a free energy

$$\mathcal{E}[\phi] = \int \frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\varepsilon^2} (1 - \phi^2)^2 dx. \quad (7.1)$$

We consider the $H^{-\alpha}$ gradient flow,

$$\frac{\partial \phi}{\partial t} = -m(-\Delta)^\alpha \left(-\Delta \phi - \frac{1}{\varepsilon^2} \phi(1 - \phi^2) \right) + f(t), \quad \alpha = 0 \quad \text{or} \quad 1, \quad (7.2)$$

where f is the given source term. When $\alpha = 0$, (7.2) is the standard Allen-Cahn equation; when $\alpha = 1$, it becomes the standard Cahn-Hilliard equation.

Example 1. In the first example, we validate the convergence order of the new schemes. Considering a two-dimensional domain $(0, 2)^2$ with periodic boundary conditions, let $\alpha = 0$, $m = \varepsilon = 0.2$ in (7.2) and f is chosen such that the exact solution of (7.2) is

$$\phi(x, y, t) = e^{\sin(\pi x) \sin(\pi y)} \sin(t). \quad (7.3)$$

We use the Fourier Galerkin method with $Nx = Ny = 40$ in space so that the spatial discretization error is negligible compared to the time discretization error. In Fig. 6, we plot the convergence rate of the L^2 error at $T = 1$ by using the second- to fourth- order schemes (2.11). We observe the expected convergence order for all the cases with different β . We also observe that for the same order, the error increases slightly with larger β .

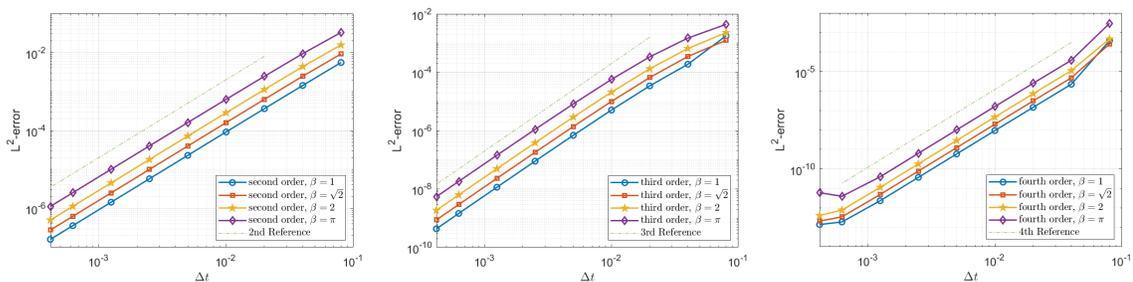


FIGURE 6. Convergence test for the general IMEX type methods. From left to right: second order, third order and fourth order schemes with different β .

Example 2. In the second example, we solve a benchmark problem for the Allen-Cahn equation [12]. Consider a two-dimensional domain $(-128, 128)^2$ with a circle of radius $R_0 = 100$. In other words, the initial condition is given as

$$\phi(x, y, 0) = \begin{cases} 1, & x^2 + y^2 < 100^2, \\ -1, & x^2 + y^2 \geq 100^2. \end{cases} \quad (7.4)$$

By mapping the domain to $(-1, 1)^2$, the parameters in (7.2) are given by $m = 6.10351 \times 10^{-5}$, $\varepsilon = 0.0078$, $\alpha = 0$ and $f = 0$. In the sharp interface limit, the radius at time t is given by

$$R = \sqrt{R_0^2 - 2t}. \quad (7.5)$$

We use the Fourier Galerkin method with $Nx = Ny = 512$ in space. Then we fix $\Delta t = 0.75$, which is the maximum time step we can use for the classical second-order scheme to get acceptable numerical results, and use (2.11) with different orders and different β . We plot the computed radius $R(t)$ in Fig. 7, which shows that we can use higher-order schemes with the same large time step as the second-order schemes by choosing $\beta > 1$. More importantly, we can get much more accurate results with higher-order schemes. Here, $k = 1, \beta = 1$ represents the usual first-order scheme.

Example 3. In the third example, we consider the Cahn-Hilliard equation in a two-dimensional domain $(0, 1)^2$ with periodic boundary condition and let $\alpha = 1$, $m = 1$, $\varepsilon = 0.02$ in (7.2). The initial condition is given as $\phi(0) = 0.2 + r$ and r is a random perturbation variable with uniform distribution in $[-0.02, 0.02]$. We use the Fourier Galerkin method with $Nx = Ny = 128$ in space. In Fig. 8, we compare the first- to the fourth-order schemes with different β , the reference solution is generated by using the classical fourth-order scheme with sufficiently small time step $\Delta t = 5 \times 10^{-9}$.

Several observations are in order:

- 1. We take $\Delta t = 7.5 \times 10^{-8}$ which is the maximum allowable time step for the classical second-order scheme, and observe in Fig. 8(a) that we can use the same time step for the higher-order schemes by choosing a suitable $\beta > 1$, and obtain more accurate results.

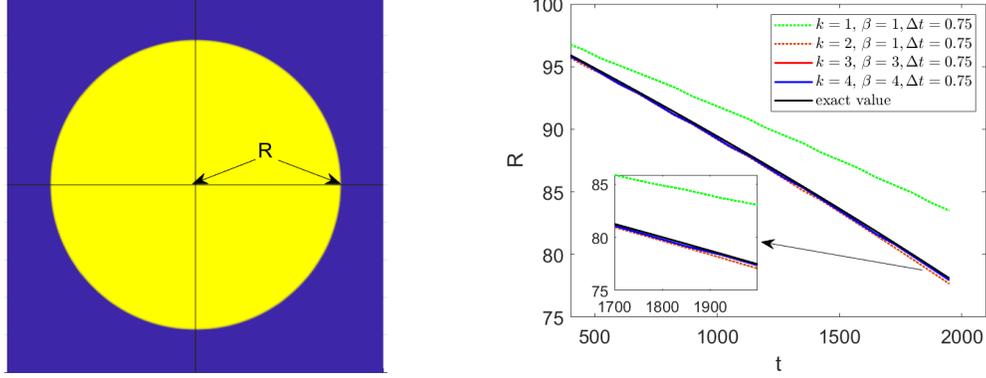
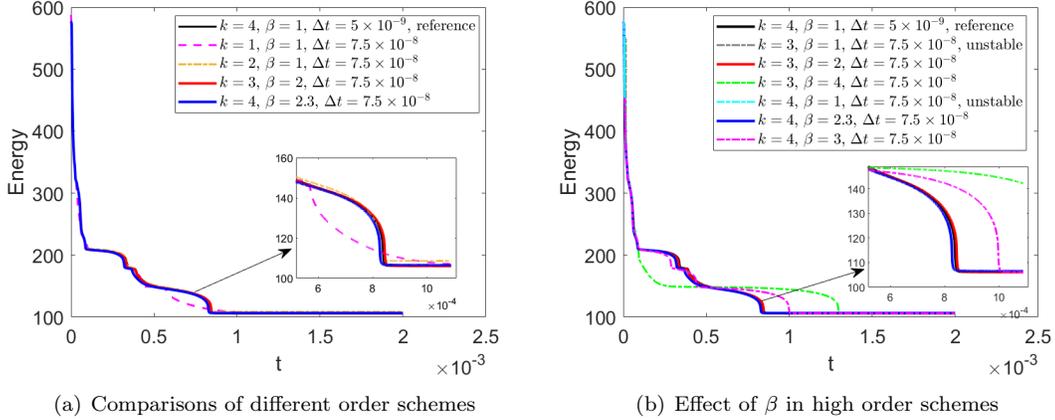


FIGURE 7. The evolution of radius R with $\Delta t = 0.75$ under different schemes.

- 2. We observe in Fig. 8(b) that the usual third- and fourth-order schemes with $\beta = 1$ are unstable, but we can get correct solutions with the third- and fourth-order schemes by choosing a suitable $\beta > 1$.
- 3. We also observe in Fig. 8(b) that β too large may lead to inaccurate results due to larger truncation errors.



(a) Comparisons of different order schemes

(b) Effect of β in high order schemes

FIGURE 8. Comparisons of different order schemes with different β for the Cahn-Hilliard equation

8. CONCLUDING REMARKS

We presented in this paper a new class of BDF and IMEX schemes for parabolic type equations based on the Taylor expansion at time $t^{n+\beta}$ with $\beta > 1$ being a tunable parameter. The new schemes are a simple generalization of the classical BDF or IMEX schemes with essentially the same computational efforts. However, they enjoy a remarkable property that their stability regions increase as the parameter β increases, making it possible, by choosing a suitably large β , to use high-order schemes with larger time steps that are only allowed with lower-order classical schemes. We also identified an explicit uniform multiplier for the new schemes of second- to fourth-order, and carried out a rigorous stability and error analysis by using the energy argument. We also presented numerical examples to show the benefit of using higher-order schemes with a suitable $\beta > 1$.

This class of new BDF and IMEX schemes makes it possible to use higher-order schemes for highly stiff systems with reasonably large time steps, and can be easily implemented with a minimal effort by modifying the code based on the classical BDF or IMEX schemes. Thus, it provides a much needed improvement on the stability of higher-order schemes. The idea behind the new class of BDF and IMEX schemes is very simple but original, and can be extended to other type of numerical schemes.

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