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Unconditionally stable difference methods for delay partial differential equations

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Abstract This paper is concerned with the numerical solution of parabolic partial differential equations with time-delay. We focus in particular on the delay dependent stability analysis of difference methods that use a non-constrained mesh, i.e., the time step-size is not required to be a submultiple of the delay. We prove that the fully discrete system unconditionally preserves the delay dependent asymptotic stability of the linear test problem under consideration, when the following discretization is used: a variant of the classical second-order central differences to approximate the diffusion operator, a linear interpolation to approximate the delay argument, and, finally, the trapezoidal rule or the second-order backward differentiation formula to discretize the time derivative. We end the paper with some numerical experiments that confirm the theoretical results.

Keywords delay partial differential equations · delay dependent stability · trapezoidal rule · backward differentiation formula · unconditional stability

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1 Introduction

Complex phenomena in biological, chemical and physical systems can sometimes be modeled by delay partial differential equations (PDEs). Since the

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1970s, such equations have been widely studied and several important properties such as existence and stability of the solution are nowadays fairly well understood, see [23]. However, the exact solution is not available in general, so one has to resort to numerical methods when solving such equations. The numerical analysis of computational methods for delay PDEs has not received too much attention yet in the literature. For some early results, we refer, for example, to the paper by van der Houwen, Sommeijer and Baker [12] who considered predictor-corrector methods for parabolic equations with delay. Higham and Sardar [11] discussed the stability of fixed points for a discretized reaction-diffusion equation with delay and found that a small delay increases the stability range. Zubik-Kowal and Vandewalle [27] investigated the convergence of waveform relaxation methods for solving semi-discrete delay PDEs.

Most numerical schemes for PDEs without delay can be adapted to the solution of delay PDEs, when they are combined with an appropriate interpolation procedure for the evaluation of the delay argument. However, the long time stability properties of such combinations may be surprisingly different from the analogous properties of methods for problems without delay. As we will see in §2 of this paper, there are many factors which may adversely affect the stability of discretization schemes. In order to gain some insight into the stability properties of numerical methods for delay PDEs we will adhere to the common practice of studying a representative model equation. In the discrete delay case, a typical test problem is the diffusion equation with a linear delayed reaction term:

$$\begin{cases} \dfrac{\partial u}{\partial t} = a\dfrac{\partial^2 u}{\partial x^2} + bu(t-\tau,x), \quad t>0,\ x\in\Omega=[0,L], \\ u(t,x)=g(t,x)\ , \quad t\in[-\tau,0]\ , \quad x\in\Omega, \\ u(t,x)=0\ , \quad t>0\ , \quad x=0 \text{ or } L. \end{cases} \tag{1}$$

This equation is a natural extension of the classical test problem in the stability analysis of parabolic PDEs. This model equation was used by Zubik-Kowal in [26], where the contractivity of θ-methods was studied. In our earlier work [14], a similar (but more general) equation was considered. For that equation, we derived the exact delay dependent stability regions of the continuous system, the semi-discrete system, and a fully discrete system. The latter was based on the Crank-Nicolson scheme on a constrained mesh, i.e., with a time stepsize that is a submultiple of delay. Wu and Gan [24] extended the above results to the case of neutral delay PDEs.

A natural follow-up to the above studies is the investigation of the stability of other classical schemes when adapted to delay PDEs. In particular, one is then looking for an answer to the following question: "*Does there exist a method which fully preserves the delay dependent asymptotic stability of PDE (1) for an arbitrary stepsize ?*" When trying to answer that question, one is inevitably confronted with the analogous question for the delay ordinary differential equation (ODE)

$$y'(t) = ay(t) + by(t-\tau). \tag{2}$$

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The delay-dependent stability properties of many classical time-integration methods applied to (2) have been investigated over the years, see the monographs [2,5] and the extensive bibliography therein. In the case of real coefficients, for example, several classes of Runge-Kutta methods, including A-stable theta methods, Gauss methods and Radau methods, are proved to preserve the delay-dependent stability of equation (2) (cf. [7–9,13]). Linear multistep methods, and backward differentiation formulae in particular, are considered in [4, 16]. Equations with complex coefficients are studied in [10,19]. Many of these results apply to some extent to (1), or at least to a semi-discrete version of that equation after an appropriate spatial discretization is employed. Nevertheless, most of these results also suffer from the limitation of a constrained mesh. To our knowledge, the delay dependent stability of numerical methods with an arbitrary stepsize for (2) is largely an open problem, too. It should be pointed out that the delay-*independent* stability of numerical methods is another matter, which is fairly well understood. For example, it is known that all A-stable natural Runge-Kutta methods preserve the delay-independent stability of delay ODEs with constant coefficients [25,17]. If the equi-stage interpolation procedure introduced by in't Hout [15] is employed in order to approximate the delay argument, stability also holds for non-constrained meshes [15,20]. The same is true for linear multistep methods [3,22].

In this paper we focus on the delay dependent stability analysis of numerical methods with a non-constrained mesh. A feasible approach for proving the unconditional stability of numerical methods with an interpolation procedure is established. A positive answer to the above question is obtained. The paper is organized as follows. In §2, we first summarize some factors which possibly affect the stability of discretization schemes. Then, in §3, we look for methods which unconditionally preserve the stability of the test problem (1). We will prove that the trapezoidal rule and the second order backward differentiation formula (BDF), combined with an appropriate spatial discretization, possess this property. In §4, we present some numerical experiments to show the difference between unconditionally stable methods and other methods. We conclude with some remarks in §5.

2 Sources of instability

There is a vast literature on the stability of difference methods for PDEs without delay and many schemes are known to be unconditionally stable for the model equation

$$\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2}, \tag{3}$$

with $a > 0$; see, e.g., [21]. However, when these methods are adapted to delay PDEs, there are several factors which possibly lead to instability. In this section, we summarize some of them.

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2.1 Stability of the continuous problem

It is well known that the model equation (3) is asymptotically stable if and only if the coefficient a is positive. In the case of delay PDEs, however, the stability condition is much more complicated. Without loss of generality, we assume $\tau = 1$ and $L = \pi$ in (1) such that the notations can be greatly simplified, i.e., the model equation reduces to

$$\begin{cases} \dfrac{\partial u}{\partial t} = a\dfrac{\partial^2 u}{\partial x^2} + bu(t-1,x), \quad t>0,\ x \in \Omega = [0,\pi], \\ u(t,x) = g(t,x)\ , \quad t \in [-1,0]\ , \quad x \in \Omega, \\ u(t,x) = 0\ , \quad t > 0\ , \quad x = 0 \text{ or } \pi, \end{cases} \tag{4}$$

where $a, b \in \mathbb{R}$. Taking the Fourier transform, we are led to the characteristic equation

$$\lambda = -ak^2 + b\mathrm{e}^{-\lambda}\ , \ k = 1, 2, \ldots; \tag{5}$$

see, e.g., [23, Ch. III]. Equation (4) is asymptotically stable for any initial function $g(t,x)$ if and only if all the roots of each of the equations (5) have negative real parts. The set of such parameter pairs (a,b) constitutes the so-called asymptotic stability region, which we denote by S_*. Using the root locus technique, one arrives at the following well-known result (cf., e.g., [6,23,14]).

Proposition 1 *The pair $(a,b) \in S_*$ if and only if $a \geq 0$ and $-a < -b < \frac{\theta}{\sin\theta}$ where θ is the root of the equation $\theta\cos\theta = -a\sin\theta$ that satisfies $\pi/2 \leq \theta < \pi$.*

The stability region S_* is drawn in Figure 1. It is bounded above by the line $C_* = \{(a,b) :\ a = b\}$; it is bounded below by the curve

$$C_0 = \left\{(a,b) :\ a(\theta) = \frac{-\theta\cos\theta}{\sin\theta} \text{ and } b(\theta) = \frac{-\theta}{\sin\theta},\ \theta \in [\frac{\pi}{2},\pi)\right\}, \tag{6}$$

and it is bounded at the left by the line segment

$$D_0 = \left\{(a,b) : a = 0,\ -\frac{\pi}{2} < b < 0\right\}.$$

Note that $D_0 \subset S_*$. In the picture it can also be seen that the wedge region defined by $a - |b| > 0$ is a strict subset of S_*. This fact can be proven easily by using (5).

An equivalent expression for S_* is given in the theorem below. It will simplify the comparison of the analytical and numerical stability regions in our subsequent stability analysis further on in this text.

Theorem 1 *The pair $(a,b) \in S_*$ if and only if $a \geq 0$ and there exists a value $\mu \in \mathbb{R}$ such that*

$$-a + \mu b < 0 \quad \textit{and} \quad \left|\frac{b(\mu - \mathrm{e}^{-\lambda})}{\lambda - (-a+\mu b)}\right| < 1,\ \Re\lambda = 0. \tag{7}$$

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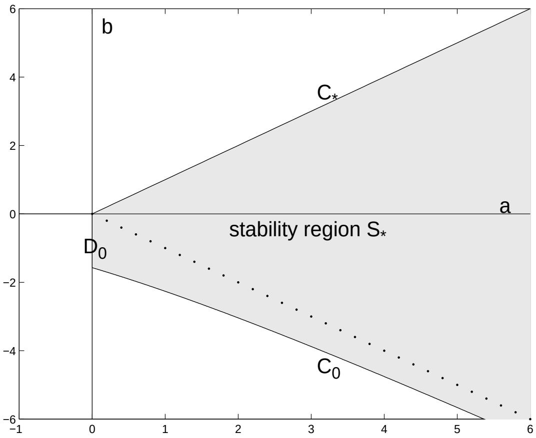

Fig. 1 Analytical stability region S_* of delay PDE (4).

Proof The pair $(a, b) \in S_*$ iff all the roots λ of (5) have negative real parts for every k. This is equivalent with the condition that $a \geq 0$ and all the roots of (5) for $k = 1$ have negative real parts. Using Theorem 1 in [13], we obtain the desired result.

2.2 Instability due to the spatial discretization

Let the spatial step size be $\Delta x = \pi/(N+1)$ for some $N \in \mathbb{Z}^+$, and define the mesh points $x_k = k\,\Delta x$ for $k = 0, 1, \ldots, N+1$. Using central differences to approximate the Laplacian we obtain the semi-discrete system

$$u_k'(t) = a\left(\frac{u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)}{\Delta x^2}\right) + b\,u_k(t-1), \qquad k = 1, \ldots, N\ ,(8)$$

where $u_k(t)$ approximates $u(t, x_k)$. It is natural now to inquire about the relationship between the stability region of the ODE system (8) and S_*. In [14] we proved that the ODE stability region is only a subset of S_*, if $a \geq 0$. In other words, the use of central differences leads to a reduction in the size of the stability region of the original delay PDE. This reduction cannot be undone by any subsequent time discretization (cf. [14, Th.3.9]).

In order to overcome this problem, an alternative central difference scheme was suggested in [14]. When Δx is replaced by $\Delta\widetilde{x} := 2\sin\frac{1}{2}\Delta x$, one obtains the corresponding (consistent) semi-discrete system

$$u_k'(t) = a\left(\frac{u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)}{\Delta\widetilde{x}^2}\right) + b\,u_k(t-1), \qquad k = 1, \ldots, N\ ,(9)$$

which has a stability region that matches exactly with S_*. In the present paper, we shall continue to use this technique in order to discretize the Laplacian operator.

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2.3 Instability due to the approximation of the delay argument

When a delay equation is solved numerically, we have to consider how to approximate the delay argument. Different approximations may lead to entirely different stability properties. For example, we consider the following scheme for (4):

$$\frac{u_k^{n+1}-u_k^n}{\Delta t}=\frac{a}{2}\frac{\delta^2 u_k^{n+1}}{\Delta\widetilde{x}^2}+\frac{a}{2}\frac{\delta^2 u_k^{n}}{\Delta\widetilde{x}^2}+bv_k^n,\ k=1,\ldots,N\,. \tag{10}$$

Here, Δt is the time stepsize; u_k^n denotes an approximation to $u(t_n,x_k)$ with $t_n=n\Delta t$; the operator δ^2 is defined by $\delta^2u_k=u_{k+1}-2u_k+u_{k-1}$, and v_k^n is an approximation to the delay argument. To ensure an as high as possible accuracy it is natural to require v_k^n to approximate $u(t_n+\frac{1}{2}\Delta t-1,x_k)$. Let $\Delta t=1/(m-\frac{1}{2})$ with $m\in\mathbb{Z}^+$, then $t_n+\frac{1}{2}\Delta t-1=t_{n-m+1}$. Hence, it seems reasonable to define

$$v_k^n=u_k^{n-m+1}. \tag{11}$$

Now we perform a discrete von Neumann stability analysis. Substituting

$$u_k^n=\xi^n \mathrm{e}^{ijk\Delta x},\ 1\le j\le N,$$

into (10) combined with (11), we get the following equation for ξ:

$$\left(\frac{1}{\Delta t}+\frac{2a\sin^2(j\Delta x/2)}{\Delta\widetilde{x}^2}\right)\xi^m+\left(\frac{-1}{\Delta t}+\frac{2a\sin^2(j\Delta x/2)}{\Delta\widetilde{x}^2}\right)\xi^{m-1}-b=0. \tag{12}$$

If $a>0$ and $b=0$, then $|\xi|<1$ so that the scheme preserves the asymptotic stability of (3). When $b\neq 0$, however, the scheme cannot completely preserve the stability of (4). In fact, for any m, there exists $a>0$, satisfying $a-|b|>0$, such that

$$\left|\frac{b}{\frac{1}{\Delta t}+\frac{2a\sin^2(\Delta x/2)}{\Delta\widetilde{x}^2}}\right|=\left|\frac{b}{m-\frac{1}{2}+\frac{1}{2}a}\right|>1.$$

This means that equation (12) has at least one root ξ lying outside of the unit disk, and thus scheme (10) is unstable. From §2.1 it is known that the wedge region defined by $a-|b|>0$ is a subset of S_*. Hence, the stability of the PDE is not preserved. Note that this instability comes from the particular approximation of the delay argument used above. An alternative approximation will be considered in Section 3.1, for which an unconditional stability result will hold.

2.4 Instability due to the time discretization

Finally, we show by means of two examples that the instability may also originate from the time discretization. To that end, we consider two unconditionally stable methods for (3). In order to exclude any adverse effects of the interpolation procedure, we shall resort here to a constrained mesh, i.e., we set

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$\Delta t = 1/m$ with $m \in \mathbb{Z}^+$. Then, every delayed argument can be evaluated from a past grid point and no interpolation procedure is necessary.

An adaptation of the Dufort-Frankel scheme to (4) leads to

$$\frac{u_k^{n+1} - u_k^{n-1}}{2\Delta t} = a \frac{u_{k+1}^n - u_k^{n+1} - u_k^{n-1} + u_{k-1}^n}{\Delta \widetilde{x}^2} + b u_k^{n-m}, \; k = 1, \ldots, N. \quad (13)$$

Setting again $u_k^n = \xi^n \mathrm{e}^{ijk\Delta x}$, we derive the equation

$$\frac{\xi - \xi^{-1}}{2\Delta t} = a \frac{2\cos j\Delta x - \xi - \xi^{-1}}{\Delta \widetilde{x}^2} + b\xi^{-m}.$$

Next, we set $\xi = -1$ and $j = N$, which leads to

$$a + (-1)^m b = 0\,.$$

This shows that, when m is even, the whole line defined by $a+b=0$ lies outside of the asymptotic stability region of scheme (13). Therefore, the scheme cannot completely preserve the stability of the underlying delay PDE (4).

Another example is the following three-level scheme:

$$\begin{aligned}\frac{u_k^{n+1} - u_k^{n-1}}{2\Delta t} &= \frac{3}{8}\Big(\frac{a}{\Delta \widetilde{x}^2}\delta^2 u_k^{n+1} + b u_k^{n+1-m}\Big) + \frac{1}{4}\Big(\frac{a}{\Delta \widetilde{x}^2}\delta^2 u_k^{n} + b u_k^{n-m}\Big) \\ &\quad + \frac{3}{8}\Big(\frac{a}{\Delta \widetilde{x}^2}\delta^2 u_k^{n-1} + b u_k^{n-1-m}\Big), \; k = 1, \ldots, N. \quad (14)\end{aligned}$$

It is obtained by applying an A-stable second-order method to the semi-discrete system (9). It is easy to verify that the scheme is stable for any $a > 0$ when $b = 0$. By means of a discrete von Neumann stability analysis, we can again show that the method cannot completely preserve the stability of (4).

These examples show that some methods which are unconditionally stable for PDE (3), are possibly no longer unconditionally stable for delay PDE (4).

3 Delay dependent stability preserving difference methods

Motivated by the above discussion and examples, we will now look for methods which completely preserve the asymptotic stability of the model equation (4).

3.1 A discretization based on the trapezoidal rule

An application of the trapezoidal rule to (9) leads to

$$\frac{u_k^{n+1} - u_k^{n}}{\Delta t} = \frac{a}{2}\frac{\delta^2 u_k^{n+1}}{\Delta \widetilde{x}^2} + \frac{a}{2}\frac{\delta^2 u_k^{n}}{\Delta \widetilde{x}^2} + \frac{b}{2}(v_k^{n+1} + v_k^n), \; k = 1, \ldots, N, \quad (15)$$

where v_k^n approximates $u(t_n - 1, x_k)$. Let $\Delta t = 1/(m - \varepsilon)$ with integer m and $\varepsilon \in [0, 1)$, then $t_n - 1 = t_{n-m} + \varepsilon \Delta t$ and we can use linear interpolation to get

$$v_k^n = \varepsilon u_k^{n-m+1} + (1 - \varepsilon) u_k^{n-m}.$$

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Substituting the above into (15), we find, after rearranging terms,

$$\frac{u_k^{n+1}-u_k^n}{\Delta t} = \frac{a}{2\Delta\widetilde{x}^2}[\delta^2 u_k^{n+1}+\delta^2 u_k^n]+\frac{b}{2}\left(\varepsilon u_k^{n-m+2}+u_k^{n-m+1}+(1-\varepsilon)u_k^{n-m}\right), \tag{16}$$

The above equation is subject to the following discrete initial and boundary conditions

$$\begin{cases} u_0^n = 0, \; n > 0, \\ u_{N+1}^n = 0, \; n > 0, \\ u_k^n = g(t_n, x_k), \; n = -m, -m+1, \ldots, 0; \; k = 0, 1, \ldots, N+1\,. \end{cases} \tag{17}$$

Since we have a zero Dirichlet boundary condition, the discrete system (16) can be solved by using finite Fourier series. Also, in this particular case the discrete von Neumann stability analysis provides a stability condition for (16) that is not only necessary but also sufficient, see, e.g., [21]. Substituting $u_k^n = \xi^n \mathrm{e}^{ijk\Delta x}$, with $j = 1, 2, \ldots, N$, into (16), we find

$$\frac{\xi-1}{\Delta t} = \frac{-2a}{\Delta\widetilde{x}^2}(\xi+1)\sin^2(j\Delta x/2)+\frac{1}{2}b\xi^{-m}(\xi+1)(1-\varepsilon+\varepsilon\xi), \; j = 1, \ldots, N. \tag{18}$$

Difference equation (16) is asymptotically stable if and only if all of the roots of each of the algebraic equations in (18) satisfy $|\xi| < 1$.

In the following, we identify the relationship between the analytical stability region S_* and the numerical stability region. The result is formulated as Theorem 2 below. Its proof and also some of the proofs further on in this paper are based on the following two lemmas. The proofs of those lemmas are elementary but quite technical, and hence deferred to the appendix.

Lemma 1 *For a given $\phi \in [0, \pi)$, let the functions $r(\varepsilon)$ and $\varphi(\varepsilon)$ be defined by*

$$1-\varepsilon+\varepsilon \mathrm{e}^{i\phi} = r(\varepsilon)\mathrm{e}^{i\varphi(\varepsilon)}, \; \varepsilon \in [0, 1], \tag{19}$$

with $\varphi(0) = 0$ and $\varphi(\varepsilon)$ continuous. Then $0 < r(\varepsilon) \le 1$, $0 \le \varphi(\varepsilon) \le \phi$ and

$$f(\varepsilon) := 2(1-\varepsilon)\tan\frac{\phi}{2}+\varphi(\varepsilon) \ge \phi. \tag{20}$$

Lemma 2 *Let $\varepsilon \in [0, 1], \phi \in [0, \pi)$, and let $\varphi(\varepsilon)$ be defined by (19). Then*

$$h(\varepsilon) := (3-\varepsilon)\sqrt{(5-3\cos\phi)(1-\cos\phi)}-3\phi+\varphi(\varepsilon) \ge 0.$$

Theorem 2 *If $(a, b) \in S_*$, then the difference equation (16) is asymptotically stable, i.e., the discrete scheme unconditionally preserves the delay dependent stability of the model equation (4).*

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Proof We need to prove that all the roots ξ of (18) for every j satisfy $|\xi| < 1$ under the assumption $(a, b) \in S_*$. We first consider the case of $j = 1$, i.e.,

$$\frac{\xi - 1}{\Delta t} = \frac{-a}{2}(\xi + 1) + \frac{1}{2} b\, \xi^{-m}(\xi + 1)(1 - \varepsilon + \varepsilon\, \xi). \qquad (21)$$

It is easy to see that, for any $a > 0$ and $b = 0$, all roots of (21) satisfy $|\xi| < 1$.

Now, assume that the statement that all roots of (21) satisfy $|\xi| < 1$ for all $(a, b) \in S_*$ does not hold true. Then, since the roots of a polynomial are continuously dependent on its coefficients, there must exist at least one point $(a_1, b_1) \in S_*$ such that (21) has a root $|\xi|$ with $|\xi| = 1$. It is easy to verify $\xi \neq -1$. Let $\xi = \mathrm{e}^{i\phi}$ with $\phi \in [0, \pi)$. A short calculation then reveals that

$$2i(m - \varepsilon) \tan \frac{\phi}{2} = -a_1 + b_1 \mathrm{e}^{-im\phi}(1 - \varepsilon + \varepsilon \mathrm{e}^{i\phi}).$$

Using the functions defined in Lemma 1, we can rewrite this as

$$2i(m - \varepsilon) \tan \frac{\phi}{2} = -a_1 + b_1 r(\varepsilon) \mathrm{e}^{-i(m\phi - \varphi(\varepsilon))}.$$

From $(a_1, b_1) \in S_*$ it follows that $(a_1, b_1 r(\varepsilon)) \in S_*$. Using Theorem 1, we conclude that there exists a real number μ such that $-a_1 + \mu b_1 r(\varepsilon) < 0$ and

$$\left| \frac{b_1 r(\varepsilon)(\mu - \mathrm{e}^{-\lambda})}{\lambda - (-a_1 + \mu b_1 r(\varepsilon))} \right| < 1, \ \Re\lambda = 0.$$

Considering

$$2i(m - \varepsilon) \tan \frac{\phi}{2} + (a_1 - \mu b_1 r(\varepsilon)) = -b_1 r(\varepsilon)(\mu - \mathrm{e}^{-i(m\phi - \varphi(\varepsilon))}),$$

and taking $\lambda = i(m\phi - \varphi(\varepsilon))$, we have

$$|2i(m - \varepsilon) \tan \frac{\phi}{2} + (a_1 - \mu b_1 r(\varepsilon))| < |i(m\phi - \varphi(\varepsilon)) + (a_1 - \mu b_1 r(\varepsilon))|,$$

which implies

$$2(m - \varepsilon) \tan \frac{\phi}{2} < m\phi - \varphi(\varepsilon).$$

This can be rearranged to

$$2(1 - \varepsilon) \tan \frac{\phi}{2} + \varphi(\varepsilon) < \phi - (m - 1)(2 \tan \frac{\phi}{2} - \phi).$$

Thus, the left-hand side is strictly smaller than ϕ, which contradicts with (20). Hence, for $j = 1$, all the roots of (18) satisfy $|\xi| < 1$ whenever $(a, b) \in S_*$.

The proof for $j = 2, \ldots, N$ follows easily. Indeed, since $(a, b) \in S_*$ implies that

$$\left(a \frac{\sin^2(j\Delta x/2)}{\sin^2(\Delta x/2)}, b \right) \in S_*,$$

by applying the conclusion just proven for $j = 1$, we arrive at the result.

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3.2 A discretization based on second order backward differentiation

Application of the second order backward differentiation formula (BDF) to (9) gives

$$\frac{3u_k^{n+2} - 4u_k^{n+1} + u_k^n}{2\Delta t} = \frac{a}{\Delta \widetilde{x}^2}\delta^2 u_k^{n+2} + bv_k^{n+2},\ k = 1, 2, \ldots, N,$$

where v_k^{n+2} is an approximation to $u(t_{n+2} - 1, x_k)$. Since $\Delta t = 1/(m - \varepsilon)$ with integer m and $\varepsilon \in [0, 1)$, we define

$$v_k^{n+2} = \varepsilon u_k^{n+3-m} + (1 - \varepsilon)u_k^{n+2-m}.$$

Therefore, we have

$$\frac{3u_k^{n+2} - 4u_k^{n+1} + u_k^n}{2\Delta t} = \frac{a}{\Delta \widetilde{x}^2}\delta^2 u_k^{n+2} + b\left((1 - \varepsilon)u_k^{n+2-m} + \varepsilon u_k^{n+3-m}\right). \quad (22)$$

In addition to the initial-boundary values (17) which are evaluated from the original PDE formulation (4), this scheme needs additional starting values $u_k^1,\ k = 1, 2, \ldots, N$. These values can be computed by means of a different scheme, e.g., the trapezoidal rule.

Next, we shall perform a discrete von Neumann stability analysis. Substituting $u_k^n = \xi^n e^{ijk\Delta x}$ into (22) yields

$$\frac{3\xi^2 - 4\xi + 1}{2\Delta t} = \frac{-4a\xi^2}{\Delta \widetilde{x}^2}\sin^2(j\Delta x/2) + b\xi^{2-m}(1 - \varepsilon + \varepsilon\xi),\ j = 1, 2, \ldots, N. \quad (23)$$

For the particular case of $j = 1$, we have

$$\frac{3 - 4\xi^{-1} + \xi^{-2}}{2\Delta t} = -a + b\xi^{-m}(1 - \varepsilon + \varepsilon\xi). \quad (24)$$

Using the same argument as the one at the end of the proof of Theorem 2, we can prove the following lemma.

Lemma 3 *If all the roots of (24) satisfy* $|\xi| < 1$ *for all* $(a, b) \in S_*$*, then all the roots of (23) satisfy* $|\xi| < 1$ *for all* $(a, b) \in S_*$ *too.*

The remainder of the paragraph is devoted to proving the central result on the stability of the BDF method.

Theorem 3 *If* $(a, b) \in S_*$*, then the difference equation (22) is asymptotically stable, i.e., the method unconditionally preserves the delay dependent stability of the model equation (4).*

Proof The proof is based on an analysis of the roots of (24) for different values of m. We split the proof into three parts which will be formulated further on as three separate lemmas. For $m = 1$ and for $m = 2$, we show correctness of the result in Lemma 4 and Lemma 5, respectively. Their proofs are based on a simple argument using the so-called boundary locus technique (cf. [1]). In this case, the stability region of (23) is easily bounded by half lines in the (a, b)-plane. The remaining values of m, i.e., $m \geq 3$, require a more elaborate proof, and shall be dealt with in a unified way in Lemma 6.

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In the case of $m = 1$, equation (24) can be reformulated as

$$(1-\varepsilon)\left(\frac{3}{2} - 2\xi^{-1} + \frac{1}{2}\xi^{-2}\right) = -a + b\xi^{-1}(1-\varepsilon+\varepsilon\xi). \tag{25}$$

For any $\varepsilon \in [0, 1)$, we define the set

$$S_1(\varepsilon) = \{(a, b) : \text{ all roots of (25) satisfy } |\xi| < 1\}.$$

Note that if $\partial S_1(\varepsilon) \cap S_*$ is empty, then necessarily $S_* \subseteq S_1(\varepsilon)$ because

$$S_1(\varepsilon) \cap S_* \supseteq \{(a, b) : a > 0\,,\ b = 0\},$$

and because ξ in (25) is continuously dependent on a and b. Also,

$$\partial S_1(\varepsilon) \subseteq \{(a, b) : \text{ (25) has at least one root } \xi \text{ with } |\xi| = 1\}.$$

Let $\xi = \mathrm{e}^{i\phi}$ in (25). Since the coefficients of (25) are real, the roots come in complex conjugate pairs. Hence,we can restrict our analysis to $\phi \in [0, \pi]$. The value $\phi = 0$, i.e., $\xi = 1$, gives

$$-a + b = 0,$$

which represents a line in the (a, b)-plane. This line is identical to the boundary C_* of the analytical stability region S_*. The value $\phi = \pi$, i.e., $\xi = -1$, gives

$$4(1-\varepsilon) = -a - b(1-2\varepsilon). \tag{26}$$

This represents another line, which we denote by C^1_π. For the other ϕ-values, we have

$$(1-\varepsilon)[(1-\cos\phi)^2 + i\sin\phi(2-\cos\phi)] = -a + b((1-\varepsilon)\cos\phi + \varepsilon - i(1-\varepsilon)\sin\phi).$$

Separating real and imaginary parts yields the set of equations

$$\begin{cases} (1-\varepsilon)(1-\cos\phi)^2 = -a + b((1-\varepsilon)\cos\phi + \varepsilon), \\ (1-\varepsilon)\sin\phi\,(2-\cos\phi) = -b(1-\varepsilon)\sin\phi. \end{cases}$$

Solving for a and b, one obtains

$$a = -((1-\varepsilon) + \varepsilon(2-\cos\phi)) \quad \text{and} \quad b = -(2-\cos\phi),$$

which represent a line segment starting at $(-1, -1)$ and ending at $(-1-2\varepsilon, -3)$. We denote this segment by C^1_ϕ. As an illustration, these lines and segments are shown in Fig. 2 for two different values of ε. Inspection of their locations leads to the following result.

Lemma 4 *For any $\varepsilon \in [0, 1)$, we have $S_* \subseteq S_1(\varepsilon)$.*

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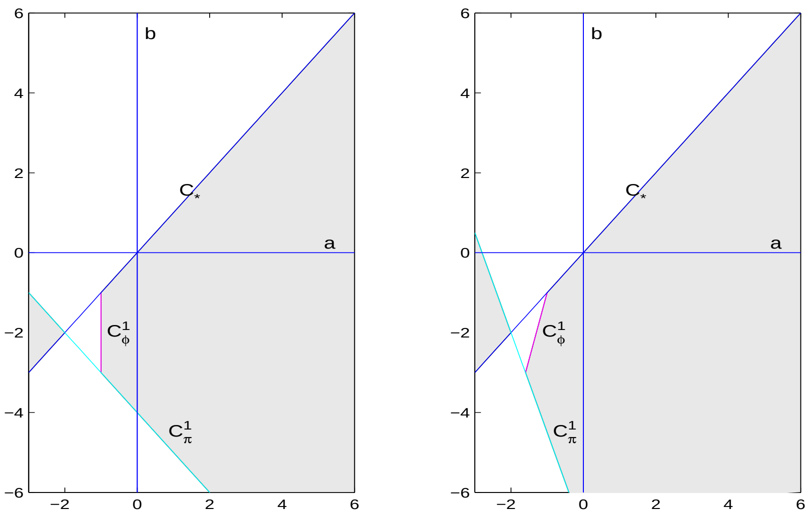

Fig. 2 Boundary locus of $S_1(\varepsilon)$. Left: $\varepsilon = 0$. Right: $\varepsilon = 0.3$.

Proof It is sufficient to prove that C^1_π and C^1_ϕ lie outside of S_*. Since C^1_ϕ lies in the left half plane, it naturally lies outside of S_*. Since C^1_π intersects the line $a = 0$ at $(0, -2 - \frac{2}{1-2\varepsilon})$ whose b-coordinate does not belong $(-\frac{\pi}{2}, 0)$, it does not intersect the boundary D_0 of S_*. Since C^1_π intersects the line $b = a$ at (-2, -2) which lies in the left half plane, it is sufficient to prove that C^1_π does not intersect the boundary C_0 of S_*. Considering that the slope of C^1_π is $\frac{-1}{1-2\varepsilon}$, it suffices to consider the limiting case $\varepsilon = 0$ and to prove that the corresponding C^1_π does not intersect C_0.

If both would intersect, substituting the parameter equations of C_0 (6) into (26) with $\varepsilon = 0$ yields

$$4 = \frac{\theta \cos\theta}{\sin\theta} + \frac{\theta}{\sin\theta} = \frac{\theta}{\tan\frac{\theta}{2}} \leq \frac{\pi}{2}, \quad \theta \in [\frac{\pi}{2}, \pi)\,.$$

This is a contradiction, which completes the proof of the lemma.

Next we deal with the case of $m = 2$. Formula (24) becomes

$$(2-\varepsilon)\left(\frac{3}{2} - 2\xi^{-1} + \frac{1}{2}\xi^{-2}\right) = -a + b\xi^{-2}(1 - \varepsilon + \varepsilon\xi). \qquad (27)$$

We define the set

$$S_2(\varepsilon) = \{(a, b) : \text{ all roots of (27) satisfy } |\xi| < 1\}.$$

We perform an analysis similar to the case of $m = 1$. Let $\xi = e^{i\phi}$ with $\phi \in [0, \pi]$. Then $\phi = 0$ gives, as before, $-a + b = 0$, i.e., a line that matches boundary C_* of S_*. The value $\phi = \pi$ leads to the line

$$4(2-\varepsilon) = -a + b(1 - 2\varepsilon), \qquad (28)$$

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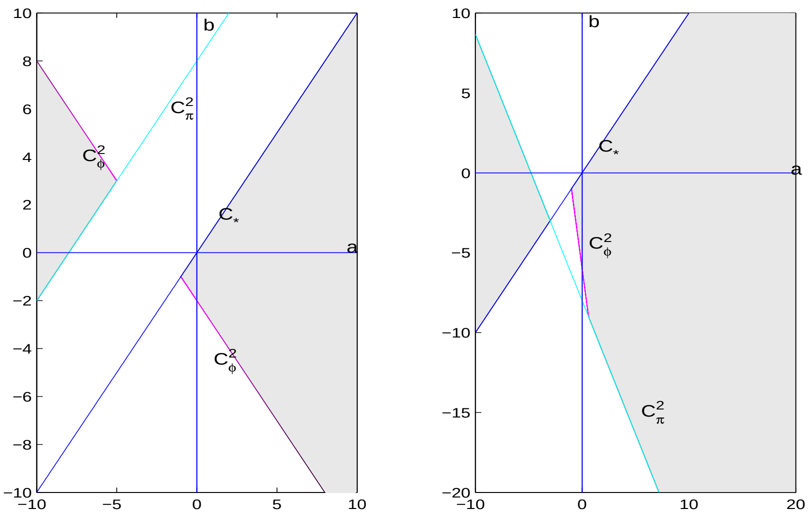

Fig. 3 Boundary locus of $S_2(\varepsilon)$. Left: $\varepsilon = 0$. Right: $\varepsilon = 0.8$.

which we denote by C_π^2. For the other ϕ-values, equation (27) can be written as a two by two linear system of equations, the solution of which is given by

$$a = \frac{(\varepsilon-1)(3\varepsilon-4)(1-\cos\phi)}{2(1-\varepsilon)\cos\phi+\varepsilon} - 1 \quad \text{and} \quad b = \frac{(3\varepsilon-4)(1-\cos\phi)}{2(1-\varepsilon)\cos\phi+\varepsilon} - 1\,.$$

This is the parameterization of a line segment in the (a, b)-plane, starting at (-1, -1) and ending in $(\frac{(2-\varepsilon)(6\varepsilon-5)}{2-3\varepsilon}, \frac{3(2-\varepsilon)}{2-3\varepsilon})$. We denote this line segment by C_ϕ^2. Note that C_ϕ^2 goes through (∞, ∞) when $\varepsilon \le \frac{2}{3}$. Also, C_ϕ^2 is part of the line defined by

$$(b+1)(1-\varepsilon) + a + 1 = 0. \tag{29}$$

We draw these lines in Fig. 3 for two different values of ε. An analysis of their locations yields the following result.

Lemma 5 *For any* $\varepsilon \in [0, 1)$*, we have* $S_* \subseteq S_2(\varepsilon)$.

Proof With a similar line of reasoning as in the proof of Theorem 4, we shall show that C_π^2 and C_ϕ^2 lie outside of S_*. First, we consider C_ϕ^2 and actually prove the stronger result that the entire line defined by (29) lies outside of S_*. Obviously, this line intersects C_* only at (-1, -1). If it would intersect C_0, we could substitute the formulas for a and b from (6) into (29), and find, for some $\theta \in [\frac{\pi}{2}, \pi)$:

$$(1 - \frac{\theta}{\sin\theta})(1-\varepsilon) - \frac{\theta\cos\theta}{\sin\theta} + 1 = 0\,.$$

This can be rewritten as

$$2 - \varepsilon = \frac{\theta(1+\cos\theta)}{\sin\theta} - \varepsilon\frac{\theta}{\sin\theta} \le \frac{\pi}{2} - \frac{\pi}{2}\varepsilon,$$

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which contradicts with $\varepsilon \in [0, 1)$. In addition, substituting $a = 0$ into (29), we get

$$b = \frac{-1}{1-\varepsilon} - 1 \leq -2.$$

This means that line (29) does not intersect D_0.

A similar analysis for C_π^2 shows that C_π^2 lies outside of S_*. Therefore, the boundary of $S_2(\varepsilon)$ lies outside of S_* and, thus, $S_* \subseteq S_2(\varepsilon)$. This completes the proof of the lemma.

Finally, we have arrived at the case of $m \geq 3$. We can prove the corresponding result below.

Lemma 6 *If $(a, b) \in S_*$, $\varepsilon \in [0, 1)$ and $m \geq 3$, then all roots ξ of (24) satisfy $|\xi| < 1$.*

Proof Assume that the conclusion of the theorem is not true, then there exists a point $(a_1, b_1) \in S_*$ such that (24) has a root ξ with $|\xi| = 1$ for some $m \geq 3$.

Let $\xi = \mathrm{e}^{i\phi}$ with $\phi \in [0, \pi]$. We first prove that $\phi \neq \pi$. In fact, if $\phi = \pi$, then

$$4(m - \varepsilon) = -a_1 + (-1)^m b_1(1 - 2\varepsilon).$$

If m is odd, the above equality implies that (a_1, b_1) lies on the left-hand side of the line C_π^1. This contradicts with the fact that S_* lies on the right-hand side of C_π^1. If m is even, then (a_1, b_1) lies on the left-hand side of the line C_π^2. This also contradicts with the fact that S_* lies on the right-hand side of C_π^2.

Next we consider the case of $\phi \in [0, \pi)$ and show that this also leads to a contradiction. Substituting $\xi = \mathrm{e}^{i\phi}$ into (24) and using Lemma 1, we get

$$(m-\varepsilon)\left((1 - \cos\phi)^2 + i\sin\phi\,(2 - \cos\phi)\right) = -a_1 + b_1 r(\varepsilon)\mathrm{e}^{-i(m\phi - \varphi(\varepsilon))}. \quad (30)$$

Also, $(a_1, b_1) \in S_*$ implies $(a_1, b_1 r(\varepsilon)) \in S_*$. By Theorem 1, there exists a real number μ such that $-a_1 + \mu b_1 r(\varepsilon) < 0$ and

$$\left|\frac{b_1 r(\varepsilon)(\mu - \mathrm{e}^{-\lambda})}{\lambda - (-a_1 + \mu b_1 r(\varepsilon))}\right| < 1, \ \Re\lambda = 0. \quad (31)$$

Equation (30) can be reformulated as

$$\begin{aligned}&(m-\varepsilon)\left((1-\cos\phi)^2 + i\sin\phi\,(2-\cos\phi)\right) + (a_1 - \mu b_1 r(\varepsilon))\\ &= -b_1 r(\varepsilon)(\mu - \mathrm{e}^{-i(m\phi - \varphi(\varepsilon))}).\end{aligned}$$

We denote the left-hand side of the equation by G. Taking $\lambda = i(m\phi - \varphi(\varepsilon))$, we can use (31) to show that G is bounded as follows:

$$|G|^2 < |i(m\phi - \varphi(\varepsilon)) + (a_1 - \mu b_1 r(\varepsilon))|^2.$$

Since $a_1 - \mu b_1 r(\varepsilon) > 0$, we can work this out to get

$$(m - \varepsilon)\sqrt{(5 - 3\cos\phi)(1 - \cos\phi)} < m\phi - \varphi(\varepsilon),$$

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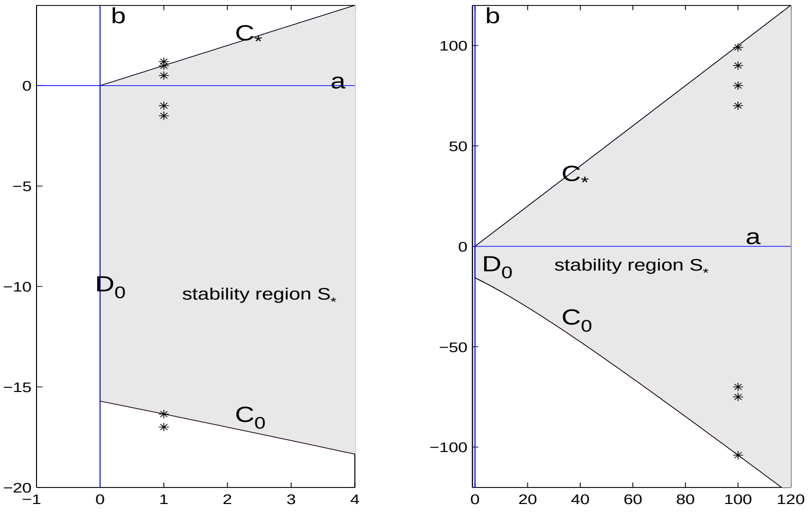

Fig. 4 Analytical stability region and location of the selected parameter pairs (a, b) (starred points) considered in the numerical experiments, for $\tau = 0.1$. Left: $a = 1$. Right: $a = 100$.

or, with $h(\varepsilon)$ as defined in Lemma 2,

$$(m-3)(\sqrt{(5-3\cos\phi)(1-\cos\phi)}-\phi)+h(\varepsilon)<0.$$

Since $\sqrt{(5-3\cos\phi)(1-\cos\phi)} \geq \phi$ for all $\phi \in [0, \pi)$, the above inequality contradicts the result of Lemma 2. This completes the proof.

Remark 1 Readers familiar with the analysis for constrained meshes (cf. [9, 13]), will notice that the analysis in the present paper is much more complicated. Obviously, this is due to the fact that we focuss on non-constrained meshes (i.e., $\varepsilon \neq 0$). The case $\varepsilon = 0$ is covered also by our analysis. However, that special case could also be proven directly, with a much simpler proof.

4 Numerical tests

In this section we present some numerical experiments to illustrate our theoretical findings. To this end, we consider four methods: the trapezoidal rule (TR), the second order backward differentiation formula (BDF), the Dufort-Frankel scheme (DF) given in (13), and scheme (10) with the delay argument evaluated by (11).

We consider test problem (1) with the function $g(t, x) = 1$ and $L = \pi$. The *delay-independent* stability condition for this equation is given by $-a \leq b < a$. The (weaker) *delay-dependent* stability condition follows from the analysis in §2, after a transformation of the problem into the normalized form (4). For

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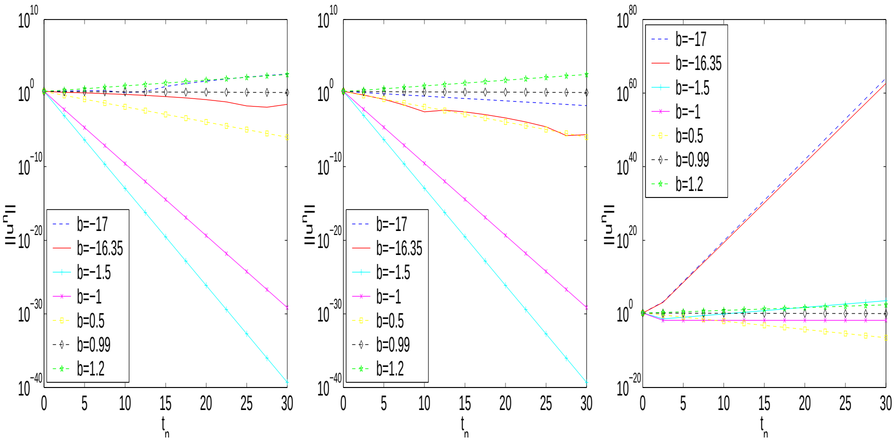

Fig. 5 The norm of the numerical solutions of TR, BDF and DF schemes with $\Delta t = 1/40$ up to $T = 30$ for $a = 1$ and different values of parameter b. Left: TR. Middle: BDF. Right: DF scheme.

example, for a delay fixed to $\tau = 0.1$, we have that for $a = 1$, the delay-dependent stability interval for the parameter b is given by $-16.35 \approx b_0 < b < 1$. For $a = 100$, the delay-dependent stability condition for the parameter b is given by $-104 \approx \widetilde{b}_0 < b < 100$ (see Fig. 4).

The effect of different spatial discretizations has been tested in our earlier work [14]. Here, we concentrate on the effect of the time discretization. The spatial step size is fixed for all our experiments to $\Delta x = \pi/50$. First, we take $a = 1$ and set time step size $\Delta t = 0.025$, i.e., $m = 4$ and $\varepsilon = 0$. In this case, the TR, BDF and DF schemes can be applied and no interpolation procedure is needed. For the tests we take $b = -17, -16.35, -1.5, -1, 0.5, 0.99, 1.2$. The corresponding (a, b) pairs are indicated as starred points on the left picture of Fig. 4. We consider the magnitude of the numerical solution at time-points t_n over a time window $[0, T]$ with $T = 30$. The observed results are given in Fig. 5, where we used the weighted discrete L_2-norm to measure the magnitude of the numerical solution:

$$\|u^n\| = \sqrt{\sum_{k=1}^{N} (u_k^n)^2 \Delta x} \ .$$

These numerical results confirm our theoretical findings. In Fig. 5 one can see that the TR and BDF schemes are stable for all $-16.35 \leq b < 1$. However, the DF scheme looses stability when $b < -1$.

Next, we take $a = 100$ and set time stepsize $\Delta t = \tau/(4 - 0.5)$, i.e., $m = 4$ and $\varepsilon = 0.5$. The results obtained with scheme (10), TR and BDF are presented in Fig. 6 for different values of parameter b. The (a, b) pairs considered in the experiments are plotted in the right picture of Fig. 4. Also Fig. 6 illustrates the stability of the TR and BDF methods, for all selected parameter values.

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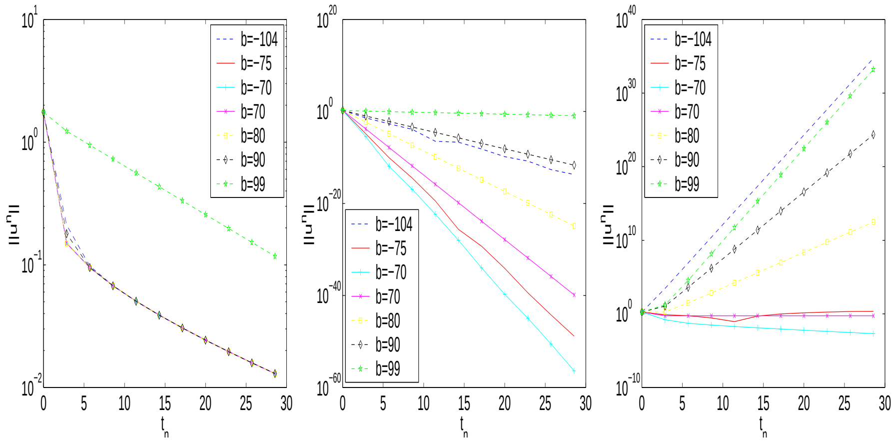

Fig. 6 The norm of the numerical solutions of TR, BDF and scheme (10) with $\Delta t = 1/35$ (i.e., $m = 4$) up to $T = 30$ for $a = 100$ and different values of parameter b. Left: TR. Middle: BDF. Right: scheme (10).

Scheme (10), however, is unstable for several values of b. The numerical results show that this scheme does not even preserve the *delay-independent* stability region.

Next, we investigate numerically the effect of different values of ε. We consider the TR and BDF schemes, and we fix $a = 100$ and $b = -104$, leading to a parameter pair just inside the stability region. Furthermore, we take $m = 4$ and $\varepsilon = 0, 0.1, 0.5, 0.8, 0.9$. The observed results are given in Fig. 7. This figure shows that both methods are stable independent of the value of ε. Note that the delay-independent stability theory cannot be applied to this situation because the parameter pair falls within the delay-dependent stability region of the PDE, but outside of the delay-independent stability region.

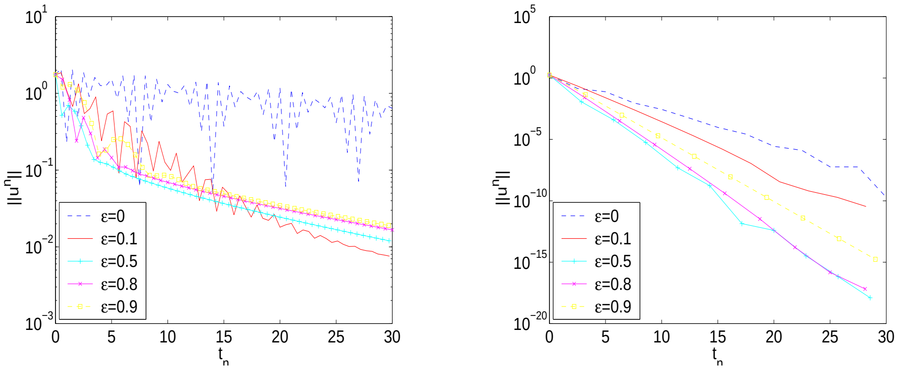

Fig. 7 The norm of the numerical solutions of TR and BDF with $\Delta t = \tau/(4 - \varepsilon)$ up to $T = 30$ for $a = 100$, $b = -104$ and different values of ε. Left: TR. Right: BDF.

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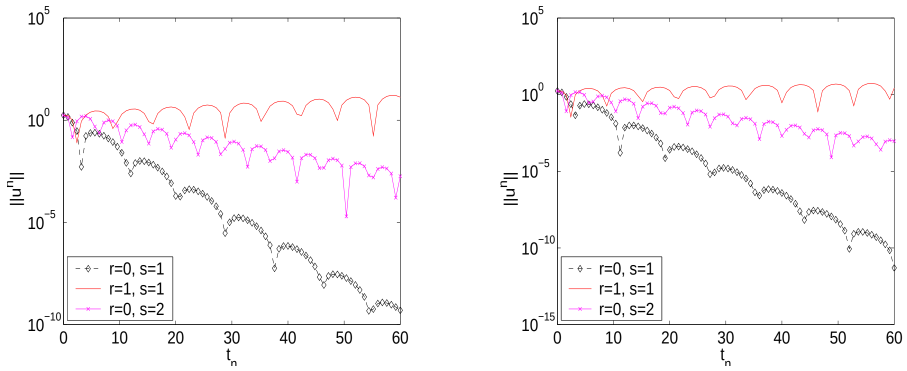

Fig. 8 The norm of the numerical solutions of G2 and R2 with $\Delta t = 1/25$ at $T = 60$ for $a = 1$, $b = -16.34$, and different types of interpolation procedure. (a) numerical solutions using G2. (b) numerical solutions using R2.

Finally, we also conducted some numerical tests with high order time discretizations for the semi-discrete system (9). These tests are not covered by our theory. We selected the 2-stage Gauss method (G2) and the 2-stage Radau IIA method (R2), which are given by the Butcher tableaus

$$\begin{array}{c|cc} 1/2-\sqrt{3}/6 & 1/4 & 1/4-\sqrt{3}/6 \\ 1/2+\sqrt{3}/6 & 1/4+\sqrt{3}/6 & 1/4 \\ \hline & 1/2 & 1/2 \end{array}\ , \qquad \begin{array}{c|cc} 1/3 & 5/12 & -1/12 \\ 1 & 3/4 & 1/4 \\ \hline & 3/4 & 1/4 \end{array}\ , \qquad (32)$$

respectively. We use a Lagrange interpolation procedure on $r+s+1$ consecutive equi-stage points around the delay point to approximate the delay argument, where r and s are non-negative integers and where s denotes the number of the used nodes behind the delay point. For example, for linear interpolation we have $r = 0$ and $s = 1$. This type of interpolation was introduced in [15]. There, it was shown that when $r \le s \le r+2$, the 2-stage Gauss and Radau methods preserve the delay-independent stability of the semi-discrete system (9) as well as the delay-independent stability of the PDE (4). We performed three experiments for different values of r and s, which all satisfy $r \le s \le r+2$. The numerical results are given in Fig. 8. These results show that in some cases the methods appear stable indeed, while in some other cases the methods are definitely unstable. So it still remains an open question whether there exist high order interpolation techniques which guarantee the delay-dependent stability.

5 Concluding remarks

In this work, we analyzed the delay dependent stability of numerical methods with an interpolation procedure. A rigorous theoretical analysis showed that both the trapezoidal rule and the second-order BDF method, combined with

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an appropriate spatial discretization, preserve the asymptotic stability characteristics of the continuous delay PDE model problem, independent of the selected time step.

The results of the paper can easily be extended to the case of multi-dimensional parabolic model problem equations. Indeed, after taking a multi-dimensional Fourier transform, the analysis of the PDE problem boils down to the analysis of a set of scalar delay equations of the form (2). However, it seems impossible to extend these results to the more general equations with both fixed and distributed delays. For θ-methods, this has been verified in [18]. The analysis of the stability of higher order time discretization methods combined with appropriate interpolation procedure remains subject of further investigation.

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Appendix: The proofs of lemmas 1 and 2

Lemma 1 *For a given $\phi \in [0, \pi)$, let the functions $r(\varepsilon)$ and $\varphi(\varepsilon)$ be defined by*

$$1 - \varepsilon + \varepsilon e^{i\phi} = r(\varepsilon) e^{i\varphi(\varepsilon)}, \ \ \varepsilon \in [0, 1], \tag{33}$$

with $\varphi(0) = 0$ and $\varphi(\varepsilon)$ continuous. Then $0 < r(\varepsilon) \le 1$, $0 \le \varphi(\varepsilon) \le \phi$ and

$$f(\varepsilon) := 2(1-\varepsilon)\tan\frac{\phi}{2} + \varphi(\varepsilon) \ge \phi. \tag{34}$$

Proof The first statement follows from $\phi \ne \pi$. A standard calculation shows

$$\varphi'(\varepsilon) = \frac{\sin\phi}{(1-\varepsilon+\varepsilon\cos\phi)^2 + \varepsilon^2\sin^2\phi} \ge 0,$$

which, when combined with $\varphi(1) = \phi$, gives the second statement. Finally, we have

$$f'(\varepsilon) = \frac{\sin\phi}{(1-2\varepsilon)^2(1-\cos^2\frac{\phi}{2}) + \cos^2\frac{\phi}{2}} - \frac{\sin\phi}{\cos^2\frac{\phi}{2}} \le 0\,,$$

which, together with $f(1) = \phi$, gives (34).

Lemma 2 *Let $\varepsilon \in [0,1], \phi \in [0, \pi)$, and let $\varphi(\varepsilon)$ be defined by (33). Then*

$$h(\varepsilon) := (3-\varepsilon)\sqrt{(5-3\cos\phi)(1-\cos\phi)} - 3\phi + \varphi(\varepsilon) \ge 0.$$

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Proof Let $\phi^* \in (0, \pi)$ be the root of the equation

$$\sqrt{(5 - 3\cos\phi)(1 - \cos\phi)} = 2\tan\frac{\phi}{2}.$$

It is easy to find that $\cos\phi^* = -1/3$, which implies that $\phi^* \in (\pi/2, \pi)$. A direct calculation shows that

$$h'(\varepsilon) = -\sqrt{(5 - 3\cos\phi)(1 - \cos\phi)} + \frac{\sin\phi}{(1 - 2\varepsilon)^2(1 - \cos^2\frac{\phi}{2}) + \cos^2\frac{\phi}{2}}.$$

If $\phi \in [0, \phi^*]$, then $h'(\varepsilon) \le 0$. Considering $\varphi(1) = \phi$ and

$$h(1) = 2(\sqrt{(5 - 3\cos\phi)(1 - \cos\phi)} - \phi) \ge 0, \ \phi \in [0, \pi],$$

we have

$$h(\varepsilon) \ge 0, \ \varepsilon \in [0, 1], \ \phi \in [0, \phi^*]. \tag{35}$$

If $\phi \in (\phi^*, \pi)$, then $h'(\varepsilon)$ has two zeros ε_1 and ε_2:

$$\varepsilon_1 < \frac{1}{2}, \ \varepsilon_2 > \frac{1}{2}, \quad \text{and} \ \frac{\varepsilon_1 + \varepsilon_2}{2} = \frac{1}{2}.$$

A further calculation shows

$$h''(\frac{1}{2}) = 0, \ h''(\varepsilon) > 0 \text{ for } \varepsilon < \frac{1}{2} \text{ and } h''(\varepsilon) < 0 \text{ for } \varepsilon > \frac{1}{2}.$$

Also, it is easy to find that

$$h(0) = 3(\sqrt{(5 - 3\cos\phi)(1 - \cos\phi)} - \phi) > 0.$$

If $\varepsilon_1 < 0$, then

$$h(\varepsilon) \ge \min\{h(0), h(1)\} > 0, \ \varepsilon \in [0, 1], \ \phi \in (\phi^*, \pi). \tag{36}$$

If $\varepsilon_1 \in [0, 1/2)$, then

$$h(\varepsilon_1) \ge (3 - \frac{1}{2})\sqrt{(5 - 3\cos\phi)(1 - \cos\phi)} - 3\phi > 0, \quad \phi \in (\phi^*, \pi) \subseteq (\pi/2, \pi),$$

and

$$h(\varepsilon) \ge \min\{h(\varepsilon_1), h(1)\} > 0, \ \varepsilon \in [0, 1], \ \phi \in (\phi^*, \pi). \tag{37}$$

A combination of (35), (36) and (37) gives the conclusion of the lemma.

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