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GALERKIN METHODS FOR PARABOLIC AND SCHRÖDINGER EQUATIONS WITH DYNAMICAL BOUNDARY CONDITIONS AND APPLICATIONS TO UNDERWATER ACOUSTICS*

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Abstract. In this paper we consider Galerkin-finite element methods that approximate the solutions of initial-boundary-value problems in one space dimension for parabolic and Schrödinger evolution equations with dynamical boundary conditions. Error estimates of optimal rates of convergence in L^2 and H^1 are proved for the associated semidiscrete and fully discrete Crank–Nicolson–Galerkin approximations. The problem involving the Schrödinger equation is motivated by considering the standard "parabolic" (paraxial) approximation to the Helmholtz equation, used in underwater acoustics to model long-range sound propagation in the sea, in the specific case of a domain with a rigid bottom of variable topography. This model is contrasted with alternative ones that avoid the dynamical bottom boundary condition and are shown to yield qualitatively better approximations. In the (real) parabolic case, numerical approximations are considered for dynamical boundary conditions of reactive and dissipative type.

Key words. linear Schrödinger evolution equation, parabolic approximation, underwater acoustics, finite element methods, error estimates, noncylindrical domain, rigid bottom boundary condition, Crank–Nicolson time stepping, parabolic equation, dynamical boundary condition

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1. Introduction. Our main goal in this paper is to analyze Galerkin-finite element methods for initial-boundary-value problems, involving dynamical boundary conditions, for the linear Schrödinger and the heat equations. In addition, in a specific problem arising in underwater acoustics and modeled by the Schrödinger equation, we will also consider an alternative boundary condition and evaluate, analytically and numerically, the two models.

We start with the underwater acoustic application. Consider the Helmholtz equation (HE) in cylindrical coordinates in the presence of cylindrical symmetry

$$\text{(HE)} \qquad \Delta p + k_0^2\,\eta^2(r,z)p = 0.$$

Here $z \geq 0$ is the depth variable increasing downwards and $r \geq 0$ is the horizontal distance (range) from a harmonic point source of frequency f_0 placed on the z axis. For simplicity we shall assume that the medium consists of a single layer of water of constant density, occupying the region $0 \leq z \leq \ell(r)$, $r \geq 0$, between the free surface

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$z = 0$ and the range-dependent bottom $z = \ell(r)$; $\ell = \ell(r)$ will be assumed to be smooth and positive. The function $p = p(r,z)$ is the acoustic pressure, $k_0 = \frac{2\pi f_0}{c_0}$ is a reference wave number, c_0 a reference sound speed, and $\eta(r,z)$ the index of refraction, defined as $\frac{c_0}{c(r,z)}$, where $c(r,z)$ is the speed of sound in the water. The (HE) is supplemented by the surface "pressure-release" condition $p(r,0) = 0$. In the case of a soft bottom the homogeneous Dirichlet boundary condition

$$\text{(D)} \qquad p = 0 \quad \text{at } z = \ell(r)$$

is assumed to hold. The case of a rigid bottom is modeled by a Neumann boundary condition (with $\dot{\ell} = \frac{d\ell}{dr}$)

$$\text{(N)} \qquad p_z - \dot{\ell}(r) p_r = 0 \quad \text{at } z = \ell(r).$$

Applying the change of variables $p(r,z) = \psi(r,z)\,\frac{e^{\mathrm{i}k_0 r}}{\sqrt{k_0 r}}$, assuming that $|2\mathrm{i}k_0\psi_r| \gg |\psi_{rr}|$ (narrow-angle paraxial approximation), and neglecting terms of $O(\frac{1}{r^2})$ (far-field approximation), we arrive (cf., e.g., [23], [19], [7]) at the standard "Parabolic" Equation (PE), which is a linear Schrödinger equation of the form

$$\text{(PE)} \qquad \psi_r = \frac{\mathrm{i}}{2k_0}\,\psi_{zz} + \mathrm{i}\,\frac{k_0}{2}\,(\eta^2(r,z) - 1)\,\psi,$$

where $\psi = \psi(r,z)$ is a complex-valued function of the two real variables r and z. The (PE) has been widely used in underwater acoustics to model one-way, long-range sound propagation near the horizontal plane of the source, in inhomogeneous, weakly range-dependent marine environments. Its solution will be sought in the domain $0 \le z \le \ell(r)$, $r \ge 0$. The (PE) will be supplemented by an initial condition $\psi(0,z) = \psi_0(z)$, $0 \le z \le \ell(0)$, modelling the source at $r = 0$, the surface boundary condition $\psi = 0$ for $z = 0$, $r \ge 0$, and a bottom boundary condition obtained by transforming (D) or (N). The Dirichlet boundary condition (D) remains of the same type ($\psi = 0$ at $z = \ell(r)$) while the Neumann boundary condition (N) is transformed to a condition of the form

$$\text{(PN)} \qquad \psi_z - \dot{\ell}(r)\,\psi_r - g_B(r)\,\dot{\ell}(r)\,\psi = 0 \quad \text{at } z = \ell(r),$$

where $g_B(r)$ is complex-valued and is usually taken simply as $\mathrm{i}\,k_0$.

The theory and numerical analysis of this initial-boundary-value problem (ibvp) with the Dirichlet bottom boundary condition is standard (cf., e.g., [20], [3]) and will not be considered any further. On the other hand the analysis is complicated in the case of the Neumann boundary condition, when $\dot{\ell}(r)$ is not the zero function, due to the presence of the term ψ_r in (PN). In [1] Abrahamsson and Kreiss proved existence and uniqueness of solutions for this problem in the case of a strictly monotone bottom, i.e., when $\dot{\ell}(r)$ is of one sign for $r \ge 0$.

We shall transform the above ibvp's to equivalent ones posed on a horizontal strip. With this aim in mind, we first introduce nondimensional variables as in [4], defined by $y := \frac{z}{L}$, $t := \frac{r}{L}$, $w := \frac{\psi}{\psi_{\mathrm{ref}}}$, where we take $L := \frac{1}{k_0}$ and $\psi_{\mathrm{ref}} := \max|\psi_0|$. Then, letting $s(t) := k_0\,\ell\big(\frac{t}{k_0}\big)$, $g(t) = k_0\,g_B\big(\frac{t}{k_0}\big)$, $\gamma(t,y) := \frac{1}{2}\left[\eta^2\big(\frac{t}{k_0}, \frac{y}{k_0}\big) - 1\right]$, we see that the (PE) becomes

$$(1.1) \qquad w_t = \frac{\mathrm{i}}{2}\,w_{yy} + \mathrm{i}\,\gamma(t,y)\,w, \quad 0 \le y \le s(t), \quad t \ge 0.$$

We note that the index of refraction η, and consequently the function γ, may be taken to be complex-valued in order to model attenuation of sound in the water. The initial condition becomes

$$w(0,y) = w_0(y) := \tfrac{1}{\psi_{\mathrm{ref}}}\,\psi_0\big(\tfrac{y}{k_0}\big), \quad 0 \le y \le s(0). \tag{1.2}$$

The surface condition remains the same, i.e.,

$$w(t,0) = 0, \quad t \ge 0, \tag{1.3}$$

while the boundary condition (PN) becomes

$$w_y(t,s(t)) - \dot{s}(t)\,\big[w_t(t,s(t)) + g(t)\,w(t,s(t))\big] = 0, \quad t \ge 0. \tag{1.4}$$

We now perform the range-dependent change of depth variable $x := \frac{y}{s(t)}$, which maps the domain of the problem onto the horizontal strip $0 \le x \le 1$, $t \ge 0$. We also make the transformation

$$u(t,x) = \exp(-\mathrm{i}\,\delta(t)x^2)\,w(t,s(t)x), \tag{1.5}$$

which defines the new field variable $u(t,x)$ for $0 \le x \le 1$, $t \ge 0$. In (1.5) $\delta(t) := \frac{\dot{s}(t)s(t)}{2}$, $t \ge 0$, where a dot denotes differentiation with respect to t. In terms of the new variables, (1.1) becomes

$$u_t = \mathrm{i}\,a(t)\,u_{xx} + \mathrm{i}\,\beta(t,x)u, \quad 0 \le x \le 1, \quad t \ge 0, \tag{1.6}$$

where, for $0 \le x \le 1$, $t \ge 0$,

$$\begin{gathered} a(t) = \tfrac{1}{2s^2(t)}, \quad \beta(t,x) = \beta_R(t,x) + \mathrm{i}\beta_I(t,x), \\ \beta_R(t,x) = \mathrm{Re}[\gamma(t,xs(t))] - \tfrac{\ddot{s}(t)s(t)x^2}{2}, \quad \beta_I(t,x) = \mathrm{Im}[\gamma(t,xs(t))] + \tfrac{\dot{s}(t)}{2\,s(t)}. \end{gathered} \tag{1.7}$$

The purpose of introducing in (1.5) the factor $e^{-\mathrm{i}\,\delta(t)x^2}$ with $\delta = \frac{\dot{s}s}{2}$ is to avoid the presence of a u_x term in the right-hand side of (1.6) and, consequently, simplify somewhat the analysis. Under the transformation (1.5), the initial and boundary conditions (1.2)–(1.4) change accordingly. Specifically, we have

$$u(0,x) = u_0(x) := e^{-\mathrm{i}\delta(0)x^2} w_0(xs(0)) \quad \forall\, x \in [0,1], \tag{1.8}$$

$$u(t,0) = 0, \quad t \ge 0, \tag{1.9}$$

and

$$u_x(t,1) = s_1(t)\,u_t(t,1) + m(t)\,u(t,1), \quad t \ge 0, \tag{1.10}$$

where

$$s_1(t) := \tfrac{\dot{s}(t)s(t)}{1+\dot{s}(t)^2}, \quad m(t) := g(t)s_1(t) + \mathrm{i}(s_1(t)\dot{\delta}(t) - 2\delta(t)), \quad t \ge 0. \tag{1.11}$$

The boundary condition (1.10) is an example of a *dynamical* boundary condition, because it involves (if $\dot{s} \ne 0$) the value of u_t at the boundary. As was already mentioned, the well posedness of ibvp's of the type $\{(1.6), (1.8), (1.9), (1.10)\}$, for t in a finite interval $[0,T]$, was proved in [1] under the assumption that $\dot{s}(t)$ is of one sign for all $t \in [0,T]$. One of our main purposes in this paper is to construct and analyze fully discrete Galerkin-finite element methods for approximating the solution of the above ibvp.

We consider the ibvp consisting of (1.6)–(1.11). We assume that the bottom is *upsloping*, i.e., that $\dot{s}(t) \le 0$, and that the problem has a unique solution, smooth enough for the purposes of the error estimation. In subsection 2.2.1 we discretize the problem in x by the standard Galerkin method and prove optimal-order L^2 and H^1 estimates for the error of the resulting semidiscretization. This is achieved by using appropriate properties of the L^2 and the elliptic projections onto the finite element subspace and a relevant H^1 superconvergence result. (The difficulty of the problem lies in the presence of the u_t term in (1.10); the condition $\dot{s}(t) \le 0$, which implies that $s_1(t) \le 0$, is needed to obtain a basic energy inequality for the error of the semidiscretization.) Subsequently, in subsection 2.2.2, we discretize the semidiscrete problem in the t variable using a Crank–Nicolson type method with a variable step-length. Again, under the assumption that $\dot{s}(t) \le 0$ for $0 \le t \le T$, we prove L^2 and H^1 error estimates which are of optimal order in x and t.

In order to overcome the analytical and numerical difficulties caused by dynamical boundary conditions of the form (1.10), Abrahamsson and Kreiss proposed in [2] an alternative rigid bottom boundary condition, which, in the case of (PE), is of the form

$$\psi_z - \mathrm{i}\, k_0\, \dot{\ell}(r)\, \psi = 0 \quad \text{at } z = \ell(r). \tag{AK}$$

This condition may be viewed as a "paraxialization" of (PN). When the nondimensionalization $z \to y$, $r \to t$, $\psi \to w$ is performed, (AK) becomes

$$w_y(t, s(t)) - \mathrm{i}\, \dot{s}(t)\, w(t, s(t)) = 0, \quad t \ge 0. \tag{1.12}$$

Finally, after changing the depth variable by $x = \frac{y}{s(t)}$ and the dependent variable by (1.5), it is not hard to see that (1.12) becomes simply

$$u_x(t, 1) = 0, \quad t \ge 0. \tag{1.13}$$

The proof of the well posedness of the ibvp consisting of (1.6)–(1.9) and (1.13) is standard, cf. [20]. Its numerical analysis too is straightforward; under no restriction on the sign of $\dot{s}(t)$ we state in subsection 2.3 optimal-order L^2 and H^1 error estimates for the standard semidiscrete Galerkin scheme and its Crank–Nicolson full discretization.

In section 3 we present results of various numerical experiments that we performed for problems on variable domains with the Neumann and Abrahamsson–Kreiss bottom boundary conditions, using the fully discrete finite element methods analyzed in section 2. We compared the results of the schemes in the case of the upsloping and downsloping rigid bottom Acoustical Society of America (ASA) wedge (a standard test problem for long range sound propagation in underwater acoustics, [16]), and found that in the upsloping case there was very good agreement between the two schemes. In the downsloping case, the scheme implementing the Neumann boundary condition was not convergent. This is in agreement with the results of Abrahamsson and Kreiss, [1], [2], who pointed out that for some downsloping bottom profiles one may observe instabilities in the case of the Neumann boundary condition. On the other hand, the scheme with the Abrahamsson–Kreiss condition was convergent and its results agreed well with those furnished by the finite difference code IFD [17], [18], [19], implemented with the rigid bottom boundary condition option. The IFD scheme uses a discretized version of the Neumann boundary condition (PN), wherein the ψ_r term is replaced by the right-hand side of the (PE). We prove a priori L^2 estimates for the resulting ibvp. A final point of interest emerging from the numerical experiments is that, for some downsloping bottom profiles $s(t)$ with an inflection point at some $t = t^*$, we observed violent growth of the L^2-norm of the numerical solution of the problem with the Neumann boundary condition for $t > t^*$. This growth (blow-up?) of the solution seems to be a feature of the problem and not an artifact of the numerical scheme.

Error estimates for a *finite difference* scheme of second-order of accuracy in x and t for some of the ibvp's considered here were proved in [4]. In the case of the Neumann boundary condition (1.10) these error estimates were shown to hold not only when $\dot{s}(t) \leq 0$ but also in the strictly downsloping case $\dot{s}(t) > 0$, $t \in [0, T]$, as a result of the validity of a certain discrete H^1 estimate; this estimate mimics an analogous H^1 estimate for the continuous problem, which holds provided $\dot{s}(t) \leq 0$ or $\dot{s}(t) > 0$ when $t \in [0, T]$. In [22] Sturm considered the Abrahamsson–Kreiss condition for the (PE) in three dimensions over a variable bottom in the more general case of a multilayered fluid medium with homothetic layers. When restricted to single layer problems in the presence of azimuthal symmetry, the scheme of [22] is similar to the one analyzed here in the case of the Abrahamsson–Kreiss bottom boundary condition. We have considerably modified the analysis of [22] and obtain optimal-order estimates, since, by using the transformation (1.5), we essentially avoid an elliptic projection with time-dependent terms. We finally mention that a uniform range step version of the scheme of this paper and also three-dimensional extensions thereof were analyzed in [5].

The problem addressed in the present paper, namely sound propagation modeled by the (PE) in a single layer of water over a rigid bottom, is, of course, an idealized model problem in underwater acoustics. More realistic environments consist, for example, of a layer of water above several layers of fluid sediments of different density, speed of sound, and attenuation overlying a rigid or soft bottom. If the layers are separated by interfaces of weakly range-dependent topography and low backscatter is expected, long-range sound propagation may again be modeled by the (PE) in each layer with transmission conditions (continuity of ψ and of $\frac{1}{\rho}\frac{\partial \psi}{\partial n}$, where ρ is the density and n the normal direction to the interface) imposed across the layer interfaces. Hence, the issue arises of how to treat the dynamical interface condition, now involving ψ_r on both sides of an interface, and the ensuing problems are analogous to those encountered in the case of the dynamical bottom boundary condition. The analysis is more complicated now, as it appears that possible nonhomotheticity of the layers has to be balanced by the jump across the interface in the imaginary part of the analog of the function γ (cf. (1.1)) in order to ensure the well posedeness of the problem [14]. For a recent review of several issues regarding the interface problem for the (PE), we refer the reader to [13]; references to underwater acoustics computations with the (PE) in the presence of interfaces with change-of-variable techniques include, e.g., [4], [22], and [13]. Here we just wish to point out that range-dependent topography has often been approximated in practice by "staircase" (piecewise horizontal) bottoms and interfaces. This raises the issue of what boundary / interface conditions to pose on the vertical part of the steps of the staircase. Moreover, it is well documented that staircase approximations lead to nonphysical energy losses or gains; cf., e.g., [16], [21]. To alleviate this problem of energy nonconservation, change-of-variable techniques may be used as in the present paper. They may also be extended to interface [13] or 3D-problems [22].

We turn now to one-dimensional (real) parabolic problems with dynamical boundary conditions. We consider the following model problem: For $0 < T < \infty$ we seek a real-valued function $u = u(t,x)$ defined for $(t,x) \in [0,T] \times [0,1]$ and satisfying

$$
\begin{aligned}
& u_t = a(t)u_{xx} + \beta(t,x)u + f(t,x) \quad \forall (t,x) \in [0,T] \times [0,1], \\
& u(t,0) = 0 \quad \forall t \in [0,T], \\
& a(t)u_x(t,1) = \varepsilon(t)\, u_t(t,1) + \delta(t)\, u(t,1) + g(t) \quad \forall t \in [0,T], \\
& u(0,x) = u_0(x) \quad \forall x \in [0,1],
\end{aligned}
\tag{1.14}
$$

where $a(t) \geq a_* > 0$ for $t \in [0,T]$ and β, f, ε, δ, g, u_0 are smooth, real-valued functions. Such problems occur in heat conduction, [12, section 4.3.5], and in other areas; see [15] for a fuller list of references. Our aim is to construct fully discrete Galerkin-finite element approximations for the ibvp (1.14) and prove error estimates, with techniques analogous to those used in the case of the Schrödinger equation. We consider two different cases depending on the sign of the function ε in the dynamical boundary condition.

We first treat the *dissipative* case, characterized by the hypothesis that $\varepsilon(t) \leq 0$ for all $t \in [0,T]$, in which the ibvp (1.14) is well posed; cf., e.g., [15]. In subsection 4.1, applying the standard Galerkin method to this case, we prove optimal-order L^2 and H^1 estimates for the error of the resulting semidiscretization and for the Crank–Nicolson–Galerkin fully discrete scheme. Matters are more complicated in the *reactive* case, wherein $\varepsilon(t) > 0$ for $t \in [0,T]$. In this case the problem is well posed in one space dimension as in the case at hand, but in general is not well posed in higher dimensions, [25], [9]. To construct a Galerkin-finite element method in this case, we replace the term u_t in the dynamical boundary condition using the pde in (1.14), thus obtaining a boundary condition involving $u_{xx}(t,1)$. The resulting ibvp is discretized in space by means of a H^1-type Galerkin method that uses finite element spaces consisting of piecewise polynomial functions in H^2 of degree at least three. In subsection 4.2 we analyze this method and prove optimal-order H^1 error estimates for the semidiscrete approximation and the fully discrete one when the Crank–Nicolson scheme is used in time-stepping. The case where $\varepsilon(t)$ changes sign in $[0,T]$ is under investigation; for a discussion, see [8].

In http://arxiv.org/abs/0904.3900v1 the interested reader may find an extended version of the present paper, [6], including proofs of results omitted herein.

2. Numerical schemes and error estimates for the (PE).

2.1. Preliminaries. Let $D := (0,1)$. We will denote by $L^2(D)$ the space of the Lebesgue measurable complex-valued functions which are square integrable on D, and by $\|\cdot\|$ the standard norm of $L^2(D)$, i.e., $\|f\| := \{\int_D |f(x)|^2\,dx\}^{\frac{1}{2}}$ for $f \in L^2(D)$. The inner product in $L^2(D)$ that induces the norm $\|\cdot\|$ will be denoted by $(\cdot,\cdot)$, i.e., $(f_1,f_2) := \int_D f_1(x)\,\overline{f_2(x)}\,dx$ for f_1, $f_2 \in L^2(D)$. Also, we will denote by $L^\infty(D)$ the space of the Lebesgue measurable functions which are bounded a.e. on D, and by $|\cdot|_\infty$ the associated norm, i.e., $|f|_\infty := \operatorname{ess\,sup}_D |f|$ for $f \in L^\infty(D)$. For $s \in \mathbb{N}_0$, we denote by $H^s(D)$ the Sobolev space of complex-valued functions having generalized derivatives up to order s in $L^2(D)$, and by $\|\cdot\|_s$ its usual norm, i.e., $\|f\|_s := \big\{\sum_{\ell=0}^{s} \|\partial_x^\ell f\|^2\big\}^{\frac{1}{2}}$ for $f \in H^s(D)$. In addition, we set $|v|_1 := \|v'\|$ for $v \in H^1(D)$. Also, $\mathbb{H}^1(D)$ will denote the subspace of $H^1(D)$ consisting of functions which vanish at $x = 0$ in the sense of trace; we set $\mathbb{H}^s(D) = H^s(D) \cap \mathbb{H}^1(D)$ for $s \geq 2$. In addition, for $s \in \mathbb{N}_0$, we denote by $W^{s,\infty}(D)$ the Sobolev space of complex-valued functions having generalized derivatives up to order s in $L^\infty(D)$, and by $|\cdot|_{s,\infty}$ its usual norm, i.e., $|f|_{s,\infty} := \max_{0\le\ell\le s} |\partial_x^\ell f|_\infty$ for $f \in W^{s,\infty}(D)$. In what follows, C will denote a generic constant independent of the discretization parameters and having in general different values at any two different places.

For later use, we recall the well known Poincaré–Friedrichs inequality

$$\|v\| \le C_{PF}\, |v|_1 \quad \forall\, v \in \mathbb{H}^1(D), \tag{2.1}$$

the Sobolev-type inequality

$$|v|_\infty \le |v|_1 \quad \forall\, v \in \mathbb{H}^1(D), \tag{2.2}$$

and the trace inequality

$$|v(1)|^2 \le 2\, \|v\|\, |v|_1 \quad \forall\, v \in \mathbb{H}^1(D). \tag{2.3}$$

Let $r \in \mathbb{N}$ and S_h be a finite dimensional subspace of $\mathbb{H}^1(D)$ consisting of complex-valued functions that are polynomials of degree less or equal to r in each interval of a nonuniform partition of D with maximum length $h \in (0, h_\star]$. It is well known [11] that the following approximation property holds:

$$\begin{aligned} &\inf_{\chi\in S_h} \left\{ \|v-\chi\| + h\|v-\chi\|_1 \right\} \le C\, h^{s+1}\, \|v\|_{s+1} \quad \forall\, v \in \mathbb{H}^{s+1}(D),\\ &\qquad\qquad\qquad\qquad\qquad\qquad s = 0, \dots, r \ \ \forall\, h \in (0, h_\star]. \end{aligned} \tag{2.4}$$

Also, we assume that the following inverse inequality holds:

$$|\phi|_1 \le C\, h^{-1}\, \|\phi\| \quad \forall\, \phi \in S_h, \quad \forall\, h \in (0, h_\star], \tag{2.5}$$

which is true when, for example, the partition of D is quasi-uniform [11]. In addition, we define the L^2-projection operator $P_h : L^2(D) \to S_h$ by

$$(P_h v, \phi) = (v, \phi) \quad \forall\, \phi \in S_h, \quad \forall\, v \in L^2(D),$$

and the elliptic projection operator $R_h : H^1(D) \to S_h$ by

$$\mathcal{B}(R_h v, \phi) = \mathcal{B}(v, \phi) \quad \forall\, \phi \in S_h, \quad \forall\, v \in H^1(D), \tag{2.6}$$

where $\mathcal{B}$ is the sesquilinear form defined for u, $w \in H^1(D)$ by $\mathcal{B}(u, w) := (u', w')$. It follows [11], [24] that

$$\begin{aligned} &\|R_h v - v\| + h\, \|R_h v - v\|_1 \le C\, h^{s+1}\, \|v\|_{s+1} \quad \forall\, v \in \mathbb{H}^{s+1}(D),\\ &\qquad\qquad\qquad\qquad\qquad\qquad s = 0, \dots, r \ \ \forall\, h \in (0, h_\star]. \end{aligned} \tag{2.7}$$

Finally, for $v \in L^2(D)$, we define the discrete negative norm

$$\|v\|_{-1,h} := \sup\left\{ \tfrac{|(v,\phi)|}{|\phi|_1} : \quad \phi \in S_h \quad \text{and} \quad \phi \neq 0 \right\} \quad \forall\, h \in (0, h_\star].$$

LEMMA 2.1. *The elliptic projection operator R_h has the following property:*

$$R_h v(1) = v(1) \quad \forall\, v \in \mathbb{H}^1(D). \tag{2.8}$$

Proof. Let $v \in \mathbb{H}^1(D)$ and ω be the element of S_h given by $\omega(x) = x$ for $x \in \overline{D}$. Then (2.6) gives $R_h v(1) - v(1) = \mathcal{B}(R_h v - v, \omega) = 0$, which is the desired result. ∎

LEMMA 2.2. *Let $\omega \in C^1(\overline{D})$. Then*

$$|P_h(\omega\phi)|_1 \le C\,|\omega|_{1,\infty}\,|\phi|_1 \quad \forall\,\phi \in S_h, \quad \forall\,h \in (0, h_\star]. \tag{2.9}$$

Proof. Let $h \in (0, h_\star]$ and $\phi \in S_h$. Since $|P_h(\omega\phi)|_1 \le |P_h(\omega\phi - R_h(\omega\phi))|_1 + |R_h(\omega\phi)|_1$, using (2.5) and (2.6) we arrive at $|P_h(\omega\phi)|_1 \le C\,h^{-1}\,\|\omega\phi - R_h(\omega\phi)\| + |\omega\phi|_1$. Next, we use the estimate (2.7) for $s = 0$ to obtain $|P_h(\omega\phi)|_1 \le C\,\big[\,|\omega|_\infty\,|\phi|_1 + |\omega'|_\infty \|\phi\|\,\big]$. Thus, the bound (2.9) follows by combining the latter inequality and (2.1). ∎

2.2. The Neumann (dynamical) boundary condition. In this subsection, we shall consider the (PE) with the Neumann boundary condition, i.e., the ibvp (1.6), (1.8), (1.9), (1.10). We shall write this problem in a slightly more general form as follows. For $T > 0$ given, we seek a function $u : [0,T] \times \overline{D} \to \mathbb{C}$ satisfying

$$(\mathcal{N}) \qquad \begin{aligned}
&u_t = \mathrm{i}\,a(t)\,u_{xx} + \mathrm{i}\,\beta(t,x)\,u + f(t,x) \quad \forall\,(t,x) \in [0,T] \times \overline{D},\\
&u(t,0) = 0 \quad \forall\,t \in [0,T],\\
&u_x(t,1) = \mu(t)\,\left[\,S(t)\,u_t(t,1) + G(t)\,u(t,1)\,\right] \quad \forall\,t \in [0,T],\\
&u(0,x) = u_0(x) \quad \forall\,x \in \overline{D}.
\end{aligned}$$

We shall assume that $a : [0,T] \to \mathbb{R}\backslash\{0\}$, $\beta,\ f : [0,T] \times \overline{D} \to \mathbb{C}$, $u_0 : \overline{D} \to \mathbb{C}$, μ, $S : [0,T] \to \mathbb{R}$, and $G : [0,T] \to \mathbb{C}$ are given functions. We shall assume that the solution u of $(\mathcal{N})$ exists uniquely, and that the data and the solution of $(\mathcal{N})$ are smooth enough for the purposes of the error estimates that will follow. (In some numerical experiments of section 3 we shall revert to the specific physical data in (1.9), (1.10), (1.11), and take the functions $a(t)$, $\beta(t,x)$ as in (1.8), $\mu(t) = \frac{\dot{s}(t)}{s(t)}$, $S(t) = \frac{s^2(t)}{1+(\dot{s}(t))^2}$, $G(t) = g(t)\,S(t) + \mathrm{i}\,[\,S(t)\,\dot{\delta}(t) - s^2(t)\,]$, where $\delta = \frac{s\dot{s}}{2}$.)

2.2.1. Semidiscrete approximation. The weak formulation of $(\mathcal{N})$, obtained by taking the $L^2(D)$ inner product of the pde in $(\mathcal{N})$ with a function in $\mathbb{H}^1(D)$, integrating by parts and using the boundary conditions, motivates defining $u_h : [0,T] \to S_h$, the semidiscrete approximation of u, by the equation

$$\begin{aligned}
(\partial_t u_h(t,\cdot), \phi) = {} & \mathrm{i}\,a(t)\,\mu(t)\,\big[\,S(t)\,\partial_t u_h(t,1) + G(t)\,u_h(t,1)\,\big]\,\overline{\phi(1)}\\
& - \mathrm{i}\,a(t)\,\mathcal{B}(u_h(t,\cdot), \phi) + \mathrm{i}\,(\beta(t,\cdot)\,u_h(t,\cdot), \phi)\\
& + (f(t,\cdot), \phi) \quad \forall\,\phi \in S_h, \quad \forall\,t \in [0,T],
\end{aligned} \tag{2.10}$$

and

$$u_h(0,\cdot) = R_h u_0(\cdot). \tag{2.11}$$

PROPOSITION 2.3. *The problem* (2.10)–(2.11) *admits a unique solution* $u_h \in C^1([0,T]; S_h)$.

Proof. Let $\dim(S_h) = J$ and $\{\phi_j\}_{j=1}^J$ be a basis of S_h consisting of real-valued functions. From (2.10), it suffices to prove that the $J \times J$ complex matrix defined by $A_{\ell j}(t) := (\phi_\ell, \phi_j) - \mathrm{i}\,a(t)\,S(t)\,\mu(t)\,\phi_\ell(1)\,\phi_j(1)$, $1 \le \ell, j \le J$, is nonsingular for

$t \in [0,T]$. Indeed, letting $t \in [0,T]$ and $x \in \mathrm{Ker}(A(t))$, we have $0 = \mathrm{Re}(\overline{x}^T A(t)x) = \|\sum_{j=1}^{J} x_j\phi_j\|^2$, and hence $x = 0$. $\square$

THEOREM 2.4. *Let u be the solution of $(\mathcal{N})$ and u_h its semidiscrete approximation defined by* (2.10)–(2.11). *Assume that $\mu(t) \le 0$ and $S(t) > 0$ for $t \in [0,T]$. Then*

$$\|u_h(t,\cdot) - u(t,\cdot)\| + h\|u_h(t,\cdot) - u(t,\cdot)\|_1 \le C\,h^{r+1}\left(\|u(t,\cdot)\|_{r+1}^2 + \int_0^t \Gamma_{\mathcal{N}}(\tau)\,d\tau\right)^{\frac{1}{2}} \tag{2.12}$$

for $t \in [0,T]$ and $h \in (0,h_\star]$, where

$$\Gamma_{\mathcal{N}}(\tau) := \|u(\tau,\cdot)\|_{r+1}^2 + \|\partial_t u(\tau,\cdot)\|_{r+1}^2 + \sum_{\ell=0}^{2}\int_0^\tau \|\partial_t^\ell u(s,\cdot)\|_{r+1}^2\,ds.$$

Proof. Let $h \in (0,h_\star]$, $\theta_h := u_h - R_h u$, and $\xi(t) := \frac{1}{a(t)}$. We first prove the H^1 superconvergence estimate

$$\|\theta_h(t,\cdot)\|_1 \le C\,h^{r+1}\left(\int_0^t \Gamma_{\mathcal{N}}(\tau)\,d\tau\right)^{\frac{1}{2}} \quad \forall\, t \in [0,T]. \tag{2.13}$$

Using (2.6) and (2.8) we obtain

$$\begin{aligned}(\partial_t\theta_h(t,\cdot),\phi) &= \mathrm{i}\,a(t)\,\mu(t)\left[S(t)\,\partial_t\theta_h(t,1) + G(t)\,\theta_h(t,1)\right]\overline{\phi(1)}\\ &\quad - \mathrm{i}\,a(t)\,\mathcal{B}(\theta_h(t,\cdot),\phi) + \mathrm{i}\,(P_h(\beta(t,\cdot)\,\theta_h(t,\cdot)),\phi)\\ &\quad + \left(\Psi_\star(t,\cdot),\phi\right) \quad \forall\,\phi \in S_h, \quad \forall\, t \in [0,T],\end{aligned} \tag{2.14}$$

where $\Psi_\star := [\partial_t u - R_h(\partial_t u)] - \mathrm{i}\,\beta\,(u - R_h u)$. Set $\phi = \partial_t\theta_h$ in (2.14) and then take imaginary parts to obtain

$$\begin{aligned}\tfrac{d}{dt}|\theta_h(t,\cdot)|_1^2 &\le |\mu(t)|\left[-2\,S^\star\,|\partial_t\theta_h(t,1)|^2 + 2\,|G(t)|\,|\theta_h(t,1)|\,|\partial_t\theta_h(t,1)|\,\right]\\ &\quad + 2\,|\xi(t)|\,\|\partial_t\theta_h(t,\cdot)\|_{-1,h}\,|P_h(\beta(t,\cdot)\,\theta_h(t,\cdot))|_1\\ &\quad + 2\,\xi(t)\,\mathrm{Im}(\Psi_\star(t,\cdot),\partial_t\theta_h(t,\cdot)) \quad \forall\, t \in [0,T],\end{aligned} \tag{2.15}$$

where $S^\star := \inf_{[0,T]} S > 0$. In order to bound properly the quantity $\|\partial_t\theta_h\|_{-1,h}$, first use (2.7) to obtain

$$\|\Psi_\star(t,\cdot)\| \le C\,h^{r+1}\left[\,\|u(t,\cdot)\|_{r+1} + \|\partial_t u(t,\cdot)\|_{r+1}\right] \quad \forall\, t \in [0,T]. \tag{2.16}$$

Then, use of (2.2) and (2.16) in (2.14) gives

$$\begin{aligned}\left|(\partial_t\theta_h(t,\cdot),\phi)\right| &\le |a(t)|\left[S(t)\,|\mu(t)|\,|\partial_t\theta_h(t,1)| + \left(\,|G(t)|\,|\mu(t)| + 1\,\right)|\theta_h(t,\cdot)|_1\right]|\phi|_1\\ &\quad + C\,h^{r+1}\left(\,\|\partial_t u(t,\cdot)\|_{r+1} + \|u(t,\cdot)\|_{r+1}\,\right)\|\phi\|\\ &\quad + |\beta(t,\cdot)|_\infty\,\|\theta_h(t,\cdot)\|\,\|\phi\| \quad \forall\,\phi \in S_h, \quad \forall\, t \in [0,T],\end{aligned}$$

which, along with (2.1), yields that

$$\begin{aligned}2\,|\xi(t)|\,\|\partial_t\theta_h(t,\cdot)\|_{-1,h} &\le C\left[\,|\theta_h(t,\cdot)|_1 + h^{r+1}\left(\,\|\partial_t u(t,\cdot)\|_{r+1} + \|u(t,\cdot)\|_{r+1}\,\right)\right]\\ &\quad + 2\,S(t)\,|\mu(t)|\,|\partial_t\theta_h(t,1)| \quad \forall\, t \in [0,T].\end{aligned} \tag{2.17}$$

Thus, combining (2.15), (2.17), (2.1), (2.2), and (2.9), we arrive at

$$\tfrac{d}{dt}|\theta_h|_1^2 \leq C\,\left[\,|\theta_h|_1^2 + h^{2(r+1)}\left(\,\|\partial_t u\|_{r+1}^2 + \|u\|_{r+1}^2\,\right)\right] + 2\,\xi\,\mathrm{Im}(\Psi_\star, \partial_t\theta_h) \quad \text{on} \quad [0,T].$$

Since $\theta_h(0,\cdot) = 0$, integrating with respect to t in the inequality above yields

$$\begin{aligned}|\theta_h(t,\cdot)|_1^2 \leq C\,&\left[\int_0^t |\theta_h(s,\cdot)|_1^2\,ds + h^{2(r+1)}\int_0^t \left(\,\|\partial_t u(s,\cdot)\|_{r+1}^2 + \|u(s,\cdot)\|_{r+1}^2\,\right)ds\right]\\ &+ \mathrm{Im}\Big\{\,2\,\xi(t)\,(\Psi_\star(t,\cdot),\theta_h(t,\cdot)) - 2\int_0^t \xi'(s)\,(\Psi_\star(s,\cdot),\theta_h(s,\cdot))\,ds\\ &- 2\int_0^t \xi(s)\,(\partial_t\Psi_\star(s,\cdot),\theta_h(s,\cdot))\,ds\Big\} \quad \forall\, t\in[0,T].\end{aligned}$$

Using in the above inequality the Cauchy–Schwarz inequality, (2.1), and (2.16), we obtain

$$|\theta_h(t,\cdot)|_1^2 \leq C\int_0^t |\theta_h(s,\cdot)|_1^2\,ds + C\,h^{2(r+1)}\,\Gamma_{\mathcal{N}}(t) \quad \forall\, t\in[0,T]. \tag{2.18}$$

The estimate (2.13) follows from (2.18) using Grönwall's lemma and (2.1). We conclude, in view of (2.7), that (2.12) holds. ∎

Taking into account the relation of a, μ, and S to the function $s(t)$ describing the bottom topography, we conclude that the error estimate of Theorem 2.4 holds in the case of domains with upsloping bottom profiles, i.e., when $\dot{s}(t) \leq 0$ for $t\in[0,T]$.

Remark 2.1. The H^1 superconvergence estimate (2.13), (2.2), and a standard L^∞ estimate for the error of the elliptic projection [26] yield as usual an optimal-order estimate of the error $|u - u_h|_\infty$ on $[0,T]$ (cf. [24]).

2.2.2. Crank–Nicolson fully discrete approximations. Let $N\in\mathbb{N}$ and $(t^n)_{n=0}^N$ be the nodes of the partition of $[0,T]$ where $t^0 = 0$, $t^N = T$, and $t^n < t^{n+1}$ for $n = 0,\dots,N-1$. Define $k_n := t^n - t^{n-1}$ for $n = 1,\dots,N$, $t^{n+\frac12} := \frac{t^n+t^{n+1}}{2}$ for $n = 0,\dots,N-1$, and $k := \max_{1\leq n\leq N} k_n$. We set $u^n := u(t^n,\cdot)$ for $n = 0,\dots,N$, where u is the solution of $(\mathcal{N})$. Finally, for sequences $(V^m)_{m=0}^M$, we define $\partial V^m := \frac{1}{k_n}(V^m - V^{m-1})$ and $\mathcal{A}V^m = \frac12(V^m + V^{m-1})$ for $m = 1,\dots,M$.

For $n = 0,\dots,N$, the Crank–Nicolson method yields an approximation $U_h^n\in S_h$ of $u(t^n,\cdot)$ as follows:

Step 1. Set

$$U_h^0 := R_h u_0. \tag{2.19}$$

Step 2. For $n = 1,\dots,N$, find $U_h^n\in S_h$ such that

$$\begin{aligned}(\partial U_h^n,\chi) &= \mathrm{i}\,a^{n-\frac12}\,\mu^{n-\frac12}\left[\,S^{n-\frac12}\,\partial U_h^n(1) + G^{n-\frac12}\,\mathcal{A}U_h^n(1)\,\right]\overline{\chi(1)}\\ &\quad - \mathrm{i}\,a^{n-\frac12}\,\mathcal{B}\big(\mathcal{A}U_h^n,\chi\big) + \mathrm{i}\,\big(\beta^{n-\frac12}\,\mathcal{A}U_h^n,\chi\big) + \big(f^{n-\frac12},\chi\big) \quad \forall\,\chi\in S_h,\end{aligned} \tag{2.20}$$

where $S^{n-\frac12} := S(t^{n-\frac12})$, $\mu^{n-\frac12} := \mu(t^{n-\frac12})$, $a^{n-\frac12} := a(t^{n-\frac12})$, $G^{n-\frac12} := G(t^{n-\frac12})$, $f^{n-\frac12} := f(t^{n-\frac12},\cdot)$, and $\beta^{n-\frac12} := \beta(t^{n-\frac12},\cdot)$.

We first examine the existence and uniqueness of U_h^n.

PROPOSITION 2.5. *Let $n \in \{1,\dots,N\}$ and suppose that $U_h^{n-1} \in S_h$ is well defined.*

(I) *If $S^{n-\frac{1}{2}} > 0$ and $\mu^{n-\frac{1}{2}} \le 0$, then there exists a constant C_n such that if $k_n < C_n$, then U_h^n is well defined by (2.20).*

(II) *In general, there exist constants $C_{n,1}$ and $C_{n,2}$ such that if $\frac{k_n}{h} < C_{n,1}$ and $k_n < C_{n,2}$, then U_h^n is well defined by (2.20).*

Proof. (I) Since (2.20) is equivalent to a linear system of algebraic equations with unknowns, the coefficients of U_h^n with respect to a basis of S_h, existence and uniqueness of U_h^n will follow if we show that if there is a $V \in S_h$ such that

$$\begin{aligned}\tfrac{1}{k_n}(V,\phi) &= \mathrm{i}\, a^{n-\frac{1}{2}}\,\mu^{n-\frac{1}{2}}\left[S^{n-\frac{1}{2}}\,\tfrac{1}{k_n}\,V(1) + G^{n-\frac{1}{2}}\,\tfrac{1}{2}\,V(1)\right]\overline{\phi(1)}\\ &\quad - \mathrm{i}\,\tfrac{a^{n-\frac{1}{2}}}{2}\,\mathcal{B}\big(V,\phi\big) + \tfrac{\mathrm{i}}{2}\,\big(P_h\big(\beta^{n-\frac{1}{2}}\,V\big),\phi\big) \quad \forall\,\phi\in S_h,\end{aligned} \tag{2.21}$$

then $V = 0$. Set $\phi = \frac{1}{k_n}V$ in (2.21), and then take imaginary parts and use the arithmetic-geometric mean inequality and (2.9) to obtain

$$\begin{aligned}|V|_1^2 &= \mu^{n-\frac{1}{2}}\,k_n\left[2\,S^{n-\frac{1}{2}}\left|\tfrac{V(1)}{k_n}\right|^2 + \tfrac{1}{k_n}\,\mathrm{Re}(G^{n-\frac{1}{2}})\,|V(1)|^2\right]\\ &\quad + \tfrac{k_n}{a^{n-\frac{1}{2}}}\,\mathrm{Re}(P_h(\beta^{n-\frac{1}{2}}\,V),\tfrac{V}{k_n})\\ &\le |\mu^{n-\frac{1}{2}}|\,k_n\left[-S^{n-\frac{1}{2}}\left|\tfrac{V(1)}{k_n}\right|^2 + \tfrac{|G^{n-\frac{1}{2}}|^2}{4S^{n-\frac{1}{2}}}\,|V(1)|^2\right]\\ &\quad + C\,\tfrac{|\beta^{n-\frac{1}{2}}|_{1,\infty}}{|a^{n-\frac{1}{2}}|}\,k_n\,|V|_1\,\|\tfrac{V}{k_n}\|_{-1,h}.\end{aligned} \tag{2.22}$$

For $\phi \in S_h$, we use (2.21), (2.2), and (2.1) to obtain

$$\begin{aligned}\big|(\tfrac{V}{k_n},\phi)\big| &\le |a^{n-\frac{1}{2}}|\,|\mu^{n-\frac{1}{2}}|\left[S^{n-\frac{1}{2}}\left|\tfrac{V(1)}{k_n}\right| + |G^{n-\frac{1}{2}}|\,\tfrac{1}{2}\,|V(1)|\right]|\phi|_1\\ &\quad + \tfrac{1}{2}\left[|a^{n-\frac{1}{2}}| + C\,|\beta^{n-\frac{1}{2}}|_\infty\right]|V|_1\,|\phi|_1,\end{aligned}$$

which yields

$$\|\tfrac{V}{k_n}\|_{-1,h} \le |a^{n-\frac{1}{2}}|\,|\mu^{n-\frac{1}{2}}|\,S^{n-\frac{1}{2}}\left|\tfrac{V(1)}{k_n}\right| + C_E\,|V|_1, \tag{2.23}$$

where $C_E := \frac{1}{2}\left[|a^{n-\frac{1}{2}}| + C\,|\beta^{n-\frac{1}{2}}|_\infty + |a^{n-\frac{1}{2}}|\,|\mu^{n-\frac{1}{2}}|\,|G^{n-\frac{1}{2}}|\right]$. Using (2.22) and (2.23), (2.2) gives

$$|V|_1^2\left\{1 - k_n\left[\tfrac{|\mu^{n-\frac{1}{2}}|\,|G^{n-\frac{1}{2}}|^2}{4S^{n-\frac{1}{2}}} + \tfrac{C\,C_E\,|\beta^{n-\frac{1}{2}}|_{1,\infty}}{|a^{n-\frac{1}{2}}|} + \tfrac{C^2}{4}\,|\mu^{n-\frac{1}{2}}|\,S^{n-\frac{1}{2}}\,|\beta^{n-\frac{1}{2}}|_{1,\infty}^2\right]\right\} \le 0, \tag{2.24}$$

which ends the proof of (I).

(II) Let $\dim S_h = J$ and $\{\phi_j\}_{j=1}^J$ be a basis of S_h consisting of real-valued functions. It is easily seen that existence and uniqueness of U_h^n is equivalent to the invertibility of a matrix $\widetilde{M} \in \mathbb{C}^{J\times J}$ defined by $\widetilde{M}_{\ell j} := \mathcal{M}(\phi_j, \phi_\ell)$ for $j,\, \ell = 1,\dots,J$, where $\mathcal{M} : S_h \times S_h \to \mathbb{C}$ is given by $\mathcal{M}(\chi,\phi) := (\chi,\phi) - \mathrm{i}\, a^{n-\frac{1}{2}}\, \mu^{n-\frac{1}{2}}\, S^{n-\frac{1}{2}}\, \chi(1)\, \overline{\phi(1)} + \frac{k_n}{2}\big[-\mathrm{i}\,(\beta^{n-\frac{1}{2}}\chi,\phi) - \mathrm{i}\ \mu^{n-\frac{1}{2}}\, a^{n-\frac{1}{2}}\, G^{n-\frac{1}{2}}\, \chi(1)\, \overline{\phi(1)} + \mathrm{i}\, a^{n-\frac{1}{2}}\, \mathcal{B}(\chi,\phi)\big]$ for $\chi,\, \phi \in S_h$. If $x \in \mathrm{Ker}(\widetilde{M})$, we have $\mathrm{Re}\big[\mathcal{M}(\phi_\star,\phi_\star)\big] = 0$ with $\phi_\star := \sum_{j=1}^{J} x_j\, \phi_j$. Then, using (2.3) and (2.5), we get

$$\begin{aligned}\|\phi_\star\|^2 &\le \tfrac{k_n}{2}\Big[\, |\beta^{n-\frac{1}{2}}|_\infty\, \|\phi_\star\|^2 + 2|\mu^{n-\frac{1}{2}}|\, |a^{n-\frac{1}{2}}|\, |G^{n-\frac{1}{2}}|\, \|\phi_\star\|\, |\phi_\star|_1 \Big]\\ &\le \tfrac{k_n}{2}\Big[\, |\beta^{n-\frac{1}{2}}|_\infty + \tfrac{C}{h}\, |\mu^{n-\frac{1}{2}}|\, |a^{n-\frac{1}{2}}|\, |G^{n-\frac{1}{2}}|\, \Big]\, \|\phi_\star\|^2,\end{aligned}$$

which, under our hypotheses, yields $x = 0$ and ends the proof of (II). ∎

Therefore, if we suppose that β is in $C([0,T], W^{1,\infty}(D))$, that $a,\ \mu,\ S,\ G$ are continuous on $[0,T]$, and that $S(t) > 0$ and $\mu(t) \le 0$ for $t \in [0,T]$ (i.e., the upsloping case), then the existence and uniqueness of U_h^n follows if $k_n \le C$, where C is a constant independent of n, since the quantity multiplying k_n in (2.24) may be uniformly bounded with respect to n. In the case of a general bottom topography, (II) shows that existence-uniqueness of U_h^n follows if we suppose that $\beta \in C([0,T], L^\infty(D))$ and $a,\ \mu,\ G$ are continuous on $[0,T]$, and take $k_n \le C_1$ and $\frac{k_n}{h} \le C_2$ for some constants $C_1,\ C_2$ independent of n.

Proposition 2.6. *Let u be the solution of $(\mathcal{N})$. For $n = 1,\dots,N$, define $\sigma^n : \overline{D} \to \mathbb{C}$ by*

$$\frac{u^n - u^{n-1}}{k_n} = \mathrm{i}\, a^{n-\frac{1}{2}}\, u_{xx}(t^{n-\frac{1}{2}},\cdot) + \mathrm{i}\, \beta^{n-\frac{1}{2}}\, \mathcal{A}u^n + f^{n-\frac{1}{2}} + \sigma^n. \tag{2.25}$$

Then,

$$\|\sigma^n\| \le C\, (k_n)^2\ B_1^n(u), \quad n = 1,\dots,N, \tag{2.26}$$

and

$$\|\sigma^{n+1} - \sigma^n\| \le C\,\big[\, (k_n)^2 + |k_{n+1} - k_n|\,\big]\, (k_n + k_{n+1})\ B_2^n(u), \quad n = 1,\dots,N-1, \tag{2.27}$$

where $B_1^n(u) := \sum_{\ell=2}^{3} \max_{[t^{n-1},t^n]} \|\partial_t^\ell u\|$ and $B_2^n(u) := \sum_{\ell=2}^{4} \max_{[t^{n-1},t^{n+1}]} \|\partial_t^\ell u\|$.

Proof. The proof follows easily by using the pde and Taylor's formula. ∎

The following theorem asserts that in the case of upsloping bottoms, the Crank–Nicolson–Galerkin method (2.19)–(2.20) yields fully discrete approximations U_h^n that converge to the solution u^n of $(\mathcal{N})$ at optimal rates in the L^2 and H^1 norms. As in the semidiscrete case this is a consequence of a H^1 superconvergence estimate for $U_h^n - R_h u(t^n,\cdot)$.

Theorem 2.7. *Let u be the solution of $(\mathcal{N})$ and $(U_h^n)_{n=0}^{N}$ be the fully discrete approximations that the method (2.19)–(2.20) produces. Assume that $\mu(t) \le 0$ and $S(t) > 0$ for $t \in [0,T]$. In addition, assume that there exists a constant $C \ge 0$ such that*

$$|k_{n+1} - k_n| \le C\, \max\big\{k_n^2, k_{n+1}^2\big\}, \quad n = 1,\dots,N-1. \tag{2.28}$$

Then, there exists a constant C_1 such that if $\max_{1\le n\le N}(k_n\, C_1) \le \frac{1}{3}$, there exists a constant $C > 0$ such that

$$\max_{1\le n\le N} \|U_h^n - R_h u^n\|_1 \le C\, (k^2 + h^{r+1})\ \Xi_{\mathcal{N}}(u) \quad \forall\, h \in (0, h_\star], \tag{2.29}$$

and

$$\max_{0\le n\le N}\|U_h^n-u^n\|_\ell \le C\,(k^2+h^{r+1-\ell})\;\Xi_N(u)\quad \forall\, h\in(0,h_\star],\;\; \ell=0,1, \tag{2.30}$$

where $\Xi_N(u) := \sum_{\ell=0}^{2}\max_{[0,T]}\|\partial_t^\ell u\|_{r+1}+\max_{[0,T]}\|\partial_t^3 u\|_1+\max_{[0,T]}\|\partial_t^4 u\|+\max_{t\in[0,T]}|\partial_t^3 u(t,1)|$.

Proof. Let $h\in(0,h_\star]$, $\theta_h^n := U_h^n - R_h u^n$ for $n=0,\dots,N$, $\xi := \frac{1}{a}$, and $\xi^{n-\frac12} := \xi(t^{n-\frac12})$ for $n=1,\dots,N$. We use (2.20), (2.25), (2.6), and (2.8) to obtain

$$\begin{aligned}(\partial\theta_h^n,\chi) &= \mathrm{i}\,a^{n-\frac12}\,\mu^{n-\frac12}\Big[S^{n-\frac12}\,\partial\theta_h^n(1)+G^{n-\frac12}\,\mathcal{A}\theta_h^n(1)-\mathcal{E}_3^n\Big]\,\overline{\chi(1)}\\ &\quad-\mathrm{i}\,a^{n-\frac12}\,\mathcal{B}(\mathcal{A}\theta_h^n,\chi)+\mathrm{i}\,(P_h(\beta^{n-\frac12}\,\mathcal{A}\theta_h^n),\chi)\\ &\quad+(\mathcal{E}_1^n-\sigma^n,\chi)+\mathrm{i}\,a^{n-\frac12}\,\mathcal{B}(\mathcal{E}_2^n,\chi)\quad\forall\,\chi\in S_h,\quad n=1,\dots,N,\end{aligned}\tag{2.31}$$

where

$$\begin{aligned}\mathcal{E}_1^n &:= \partial u^n - R_h(\partial u^n)-\mathrm{i}\,P_h[\,\beta^{n-\frac12}(\mathcal{A}u^n-R_h(\mathcal{A}u^n))\,],\\ \mathcal{E}_2^n &:= u(t^{n-\frac12})-\mathcal{A}u^n,\\ \mathcal{E}_3^n &:= S^{n-\frac12}\,\big[\,\partial_t u(t^{n-\frac12},1)-\partial u^n(1)\big]+G^{n-\frac12}\,\big[\,u(t^{n-\frac12},1)-\mathcal{A}u^n(1)\,\big].\end{aligned}$$

Using Taylor's formula and (2.7), we deduce the following estimates:

$$\|\mathcal{E}_1^n\|\le C\,h^{r+1}\left(\max_{[t^{n-1},t^n]}\|u\|_{r+1}+\max_{[t^{n-1},t^n]}\|\partial_t u\|_{r+1}\right),\tag{2.32}$$

$$|\mathcal{E}_2^n|_1\le C\,k_n^2\max_{[t^{n-1},t^n]}|\partial_t^2 u|_1,\tag{2.33}$$

and

$$|\mathcal{E}_3^n|\le C\,k_n^2\left[\max_{t\in[t^{n-1},t^n]}|\partial_t^2 u(t,1)|+\max_{t\in[t^{n-1},t^n]}|\partial_t^3 u(t,1)|\right]\tag{2.34}$$

for $n=1,\dots,N$. Set $\chi=\partial\theta_h^n$ in (2.31), and then take imaginary parts to obtain

$$\begin{aligned}|\theta_h^n|_1^2 &\le |\theta_h^{n-1}|_1^2+2\,k_n\,|\xi^{n-\frac12}|\;|P_h(\beta^{n-\frac12}\,\mathcal{A}\theta_h^n)|_1\;\|\partial\theta_h^n\|_{-1,h}\\ &\quad+k_n\,|\mu^{n-\frac12}|\,\big[\,-2\,S_\star\,|\partial\theta_h^n(1)|^2+2\,|G^{n-\frac12}|\,|\mathcal{A}\theta_h^n(1)|\,|\partial\theta_h^n(1)|\\ &\qquad\qquad+2\,|\mathcal{E}_3^n|\,|\partial\theta_h^n(1)|\,\big]\\ &\quad+2\,k_n\,\mathrm{Re}[\mathcal{B}(\mathcal{E}_2^n,\partial\theta_h^n)]+2\,k_n\,\xi^{n-\frac12}\,\mathrm{Im}(\mathcal{E}_1^n-\sigma^n,\partial\theta_h^n),\quad n=1,\dots,N,\end{aligned}\tag{2.35}$$

where $S_\star := \inf_{[0,T]} S$.

Now let us estimate $\|\partial\theta_h^n\|_{-1,h}$. For $\varphi\in S_h$, (2.31)–(2.34), (2.26), (2.2), and (2.1) give

$$\begin{aligned}|(\partial\theta_h^n,\varphi)| &\le |a^{n-\frac12}|\,|\mu^{n-\frac12}|\,S^{n-\frac12}\,|\partial\theta_h^n(1)|\,|\varphi|_1\\ &\quad+C\,|\mathcal{A}\theta_h^n|_1\,|\varphi|_1+C\,(h^{r+1}+k_n^2)\;|\varphi|_1\;\Xi_1(u),\quad n=1,\dots,N,\end{aligned}$$

where $\Xi_1(u) := \max_{[0,T]} \|u\|_{r+1} + \max_{[0,T]} \|\partial_t u\|_{r+1} + \max_{[0,T]} \|\partial_t^2 u\|_1 + \max_{[0,T]} \|\partial_t^3 u\| + \max_{t\in[0,T]} |\partial_t^3 u(t,1)|$. Hence, we conclude that

$$(2.36)\qquad \begin{aligned} 2\,k_n\,|\xi^{n-\frac12}|\,\|\partial\theta_h^n\|_{-1,h} \le 2\,k_n\,|\mu^{n-\frac12}|\,S^{n-\frac12}\,|\partial\theta_h^n(1)| + C\,k_n\,|\mathcal{A}\theta_h^n|_1 \\ + C\,k_n\,(h^{r+1}+k_n^2)\,\Xi_1(u), \quad n=1,\dots,N. \end{aligned}$$

Now, combining (2.36) and (2.35) we have

$$\begin{aligned} |\theta_h^n|_1^2 \le |\theta_h^{n-1}|_1^2 + C\,k_n\,|\mathcal{A}\theta_h^n|_1^2 + C\,k_n\,\big[\,(k_n)^4 + (h^{r+1}+k_n^2)\,|\mathcal{A}\theta_h^n|_1\,\big]\,\Xi_1(u) \\ + 2\,k_n\,\mathrm{Re}[\mathcal{B}(\mathcal{E}_2^n,\partial\theta_h^n)] + 2\,k_n\,\xi^{n-\frac12}\,\mathrm{Im}(\mathcal{E}_1^n-\sigma^n,\partial\theta_h^n), \quad n=1,\dots,N, \end{aligned}$$

from which there follows that for some constant $C_1 \ge 0$

$$\begin{aligned} (1-C_1\,k_n)\,|\theta_h^n|_1^2 \le (1+C_1\,k_n)\,|\theta_h^{n-1}|_1^2 + C_2\,k_n\,(h^{r+1}+k_n^2)^2\,(\Xi_1(u))^2 \\ + 2\,k_n\,\mathrm{Re}[\mathcal{B}(\mathcal{E}_2^n,\partial\theta_h^n)] \\ + 2\,k_n\,\xi^{n-\frac12}\,\mathrm{Im}(\mathcal{E}_1^n-\sigma^n,\partial\theta_h^n), \quad n=1,\dots,N. \end{aligned}$$

To continue, we assume that $\max_{1\le n\le N}(C_1\,k_n) \le \frac13$, which allows us to conclude that $\frac{1+C_1\,k_n}{1-C_1\,k_n} \le e^{3C_1 k_n}$ for $n=1,\dots,N$. Hence

$$\begin{aligned} |\theta_h^n|_1^2 \le e^{3C_1 k_n}\,|\theta_h^{n-1}|_1^2 + \tfrac{C_2\,k_n}{1-C_1\,k_n}\,(h^{r+1}+k_n^2)^2\,(\Xi_1(u))^2 \\ + \tfrac{2\,k_n}{1-C_1\,k_n}\Big[\,\mathrm{Re}[\mathcal{B}(\mathcal{E}_2^n,\partial\theta_h^n)] + \xi^{n-\frac12}\,\mathrm{Im}(\mathcal{E}_1^n-\sigma^n,\partial\theta_h^n)\,\Big], \quad n=1,\dots,N. \end{aligned}$$

Next, we define $\lambda_j^n := \frac{\exp\left(3C_1\sum_{\ell=j+1}^n k_\ell\right)}{1-C_1\,k_j}$ and use a simple induction argument to arrive at

$$\begin{aligned} |\theta_h^n|_1^2 \le C_2\,(\Xi_1(u))^2 \sum_{j=1}^n k_j\,\lambda_j^n\,(h^{r+1}+k_j^2)^2 \\ + 2\sum_{j=1}^n k_j\,\lambda_j^n\Big[\,\mathrm{Re}[\mathcal{B}(\mathcal{E}_2^j,\partial\theta_h^j)] + \xi^{j-\frac12}\,\mathrm{Im}(\mathcal{E}_1^j-\sigma^j,\partial\theta_h^j)\,\Big], \quad n=1,\dots,N, \end{aligned}$$

which yields

$$(2.37)\qquad |\theta_h^n|_1^2 \le C\,(h^{r+1}+k^2)^2\,(\Xi_1(u))^2 + T_A^n + T_B^n, \quad n=1,\dots,N,$$

where

$$T_A^n := 2\sum_{j=1}^n \lambda_j^n\,\mathrm{Re}\big[\,\mathcal{B}(\mathcal{E}_2^j,\theta_h^j-\theta_h^{j-1})\,\big],$$

$$T_B^n := 2\sum_{j=1}^n \lambda_j^n\,\xi^{j-\frac12}\,\mathrm{Im}(\mathcal{E}_1^j-\sigma^j,\theta_h^j-\theta_h^{j-1}).$$

Since

$$|\mathcal{E}_2^j-\mathcal{E}_2^{j+1}|_1 \le C\,(k_j+k_{j+1})\,\big[\,(k_j)^2 + |k_{j+1}-k_j|\,\big]\,\Xi_2(u), \quad j=1,\dots,N-1,$$

with $\Xi_2(u) := \max_{[0,T]} |\partial_t^2 u|_1 + \max_{[0,T]} |\partial_t^3 u|_1$ we see, after some algebra, that (2.33) and (2.28) yield

$$|T_{\scriptscriptstyle A}^n| \leq C\, k^2\, \Xi_2(u) \max_{1\leq m\leq n} |\theta_h^m|_1, \quad n = 1, \ldots, N. \tag{2.38}$$

In addition, observing that

$$|\mathcal{E}_1^j - \mathcal{E}_1^{j+1}|_1 \leq C\,(k_j + k_{j+1})\, h^{r+1}\, \Xi_3(u), \quad j = 1, \ldots, N-1,$$

with $\Xi_3(u) := \max_{[0,T]} \|\partial_t u\|_{r+1} + \max_{[0,T]} \|\partial_t^2 u\|_{r+1}$, we may see from (2.32), (2.26)–(2.28), and (2.1) that

$$|T_{\scriptscriptstyle B}^n| \leq C\,(k^2 + h^{r+1})\, \Xi_4(u) \max_{1\leq m\leq n} |\theta_h^m|_1, \quad n = 1, \ldots, N, \tag{2.39}$$

where $\Xi_4(u) := \sum_{\ell=0}^{2} \max_{[0,T]} \|\partial_t^\ell u\|_{r+1} + \sum_{\ell=3}^{4} \max_{[0,T]} \|\partial_t^\ell u\|$. Now, from (2.37), (2.38), and (2.39) it follows that

$$\begin{aligned} |\theta_h^n|_1^2 \leq{}& C\,(k^2 + h^{r+1})\,\big(\,\Xi_2(u) + \Xi_4(u)\,\big) \max_{1\leq m\leq n} |\theta_h^m|_1 \\ &+ C\,(h^{r+1} + k^2)^2\,(\Xi_1(u))^2, \quad n = 1, \ldots, N, \end{aligned}$$

which easily yields

$$\max_{0\leq n\leq N} |\theta_h^n|_1^2 \leq C\,(h^{r+1} + k^2)^2\,(\Xi_1(u) + \Xi_2(u) + \Xi_4(u))^2.$$

The desired estimate (2.29) is then a simple consequence of this inequality and (2.1). Finally, (2.30) follows from (2.29) and (2.7). ∎

2.3. The Abrahamsson–Kreiss boundary condition. We consider now the (PE) with the Abrahamsson–Kreiss bottom boundary condition, i.e., the ibvp (1.6), (1.8), (1.9), (1.12), which we rewrite here, in slightly more general form, for the convenience of the reader. For $T > 0$ given, seek a function $u : [0,T] \times \overline{D} \to \mathbb{C}$ satisfying

$$(\mathcal{AK}) \qquad \begin{aligned} &u_t = \mathrm{i}\, a(t)\, u_{xx} + \mathrm{i}\, \beta(t,x)\, u + f(t,x) \quad \forall (t,x) \in [0,T] \times \overline{D}, \\ &u(t,0) = 0 \quad \forall t \in [0,T], \\ &u_x(t,1) = 0 \quad \forall t \in [0,T], \\ &u(0,x) = u_0(x) \quad \forall x \in \overline{D}. \end{aligned}$$

We assume again that $a : [0,T] \to \mathbb{R}\backslash\{0\}$, β, $f : [0,T] \times \overline{D} \to \mathbb{C}$, $u_0 : \overline{D} \to \mathbb{C}$ are given functions. We shall assume that the solution of $(\mathcal{AK})$ exists uniquely and that the data and the solution of $(\mathcal{AK})$ are smooth enough for the purposes of the error estimation. We note that $(\mathcal{AK})$ may be considered as a special case of $(\mathcal{N})$ obtained by setting μ equal to zero in $(\mathcal{N})$. (This does not imply, of course, that we assume that $\dot{s}$ is zero. We recall that in the Abrahamsson–Kreiss formulation the effect of variable bottom enters explicitly in the definition of a and β (cf. (1.7)) and in the change-of-variable formula (1.5).) All the error estimates for $(\mathcal{AK})$ that follow may then be considered as special cases of the analogous estimates in the two preceding subsections but with some important simplifications; we shall just state the results without proofs. They imply that finite element approximations of $(\mathcal{AK})$ satisfy optimal-order error estimates under no further assumptions (except smoothness) on the shape of the bottom.

2.3.1. Semidiscrete approximation. Using the finite element subspace S_h and the notation established in subsection 2.1, we define the semidiscrete approximation u_h of the solution of $(\mathcal{AK})$ as the map $u_h : [0,T] \to S_h$ satisfying

$$(\partial_t u_h(t,\cdot),\phi) = -\mathrm{i}\, a(t)\, \mathcal{B}(u_h(t,\cdot),\phi) + \mathrm{i}\,(\beta(t,\cdot)\, u_h(t,\cdot),\phi) + (f(t,\cdot),\phi) \quad \forall\, \phi \in S_h, \quad \forall\, t \in [0,T], \tag{2.40}$$

and

$$u_h(0,\cdot) = u_h^0, \tag{2.41}$$

where $u_h^0 \in S_h$ is an approximation of u_0, which may be taken, for example, as $P_h u_0$ or $R_h u_0$.

THEOREM 2.8. *The problem* (2.40)–(2.41) *admits in* $C^1([0,T],S_h)$ *a unique solution, which in the special case* $f \equiv 0$ *and* $\beta_I \equiv 0$ *preserves the* $L^2(D)$ *norm, i.e.,* $\|u_h(t,\cdot)\| = \|u_h^0\|$ *for* $t \in [0,T]$*. In addition,*

$$\|u(t,\cdot) - u_h(t,\cdot)\|_\ell \le C \left[\|u_h^0 - R_h u_0\|_\ell + h^{r+1-\ell} \left(\|u(t,\cdot)\|_{r+1}^2 + \int_0^t \Gamma_{\mathcal{AK},\ell}(\tau)\, d\tau \right)^{\frac{1}{2}} \right]$$

for $\ell = 0,1$*,* $t \in [0,T]$ *and* $h \in (0,h_\star]$*, where* $\Gamma_{\mathcal{AK},0}(\tau) := \sum_{m=0}^{1} \|\partial_t^m u(\tau,\cdot)\|_{r+1}^2$*, and* $\Gamma_{\mathcal{AK},1}(\tau) := \Gamma_{\mathcal{N}}(\tau)$ *is the function defined in the statement of Theorem* 2.4.

2.3.2. Crank–Nicolson fully discrete approximations. We now proceed to the full discretization of $(\mathcal{AK})$ by discretizing the initial-value problem (2.40)–(2.41) in t using the Crank–Nicolson scheme. With notation introduced in subsection 2.2.2, we define for $n = 0,\dots,N$ approximations $U_h^n \in S_h$ of $u(t^n,\cdot)$, the solution of $(\mathcal{AK})$, as follows:

Step 1. Set

$$U_h^0 := u_h^0. \tag{2.42}$$

Step 2. For $n = 1,\dots,N$, find $U_h^n \in S_h$ such that

$$(\partial U_h^n,\chi) = -\mathrm{i}\, a^{n-\frac{1}{2}}\, \mathcal{B}\big(\mathcal{A}U_h^n,\chi\big) + \mathrm{i}\,\big(\beta^{n-\frac{1}{2}}\, \mathcal{A}U_h^n,\chi\big) + \big(f^{n-\frac{1}{2}},\chi\big) \quad \forall\, \chi \in S_h. \tag{2.43}$$

THEOREM 2.9. *Let* $n \in \{1,\dots,N\}$*, and suppose* U_h^{n-1} *is well defined. Then, there exists a constant* C*, independent of* n*, such that if* $k_n \le C$*,* U_h^n *is well defined by* (2.43)*. (In the special case* $f \equiv 0$ *and* $\beta_I \equiv 0$*, the scheme is conservative in* L^2*, i.e., there holds* $\|U_h^n\| = \|u_h^0\|$ *for* $n = 0,\dots,N$*.) In addition, if* $\max_{1\le n\le N} k_n$ *is sufficiently small, we have*

$$\max_{0\le n\le N} \|U_h^n - u^n\| \le C\, \big[\, \|u_h^0 - R_h u_0\| + (k^2 + h^{r+1})\, \Xi_{\mathcal{AK},0}(u) \,\big] \quad \forall\, h \in (0,h_\star],$$

where $\Xi_{\mathcal{AK},0}(u) := \sum_{m=0}^{1} \max_{[0,T]} \|\partial_t^m u\|_{r+1} + \sum_{m=2}^{3} \max_{[0,T]} \|\partial_t^m u\| + \max_{[0,T]} \|\partial_t^2 \partial_x^2 u\|$*. Also, if* (2.5) *and* (2.28) *hold, and* $\max_{1\le n\le N} k_n$ *is sufficiently small, then*

$$\max_{0\le n\le N} \|U_h^n - u^n\|_1 \le C\, \big[\, \|u_h^0 - R_h u_0\|_1 + (k^2 + h^r)\, \Xi_{\mathcal{AK},1}(u) \,\big] \quad \forall\, h \in (0,h_\star],$$

where $\Xi_{\mathcal{AK},1}(u) := \Xi_{\mathcal{AK},0}(u) + \max_{[0,T]} \|\partial_t^2 u\|_{r+1} + \max_{[0,T]} \|\partial_t^4 u\| + \max_{[0,T]} \|\partial_t^3 \partial_x^2 u\|$.

3. Numerical experiments. In this section we present the results of some numerical experiments that we performed using the fully discrete Galerkin-finite element methods, defined and analyzed in the previous section, to solve the ibvp for the (PE) in domains of variable bottom topography with Neumann and Abrahamsson–Kreiss boundary conditions. We also make, in subsection 3.2, a theoretical excursion with the aim of explaining some experimental observations made in subsection 3.1. Recall that in the case of the Neumann boundary condition, i.e., for the problem $(\mathcal{N})$, our convergence results were rigorously established in the case of upsloping bottoms, that is, when $\dot{s}(t) \leq 0$ for all $t \in [0,T]$. One of our goals in this section is to study numerically the behavior of the Neumann boundary condition in the presence of downsloping bottoms and compare the solution of $(\mathcal{N})$ with that of $(\mathcal{AK})$, for which rigorous convergence results hold for any smooth $s(t)$. In the numerical experiments the finite element subspace S_h consisted of continuous, piecewise linear functions defined on a uniform mesh, while the temporal discretization was effected with uniform time step. All computations were performed using double precision Fortran 77.

3.1. Comparison of $(\mathcal{N})$ and $(\mathcal{AK})$: The upsloping and downsloping wedge. We first consider the ASA upsloping wedge underwater acoustic test problem, see [16], with rigid bottom given in the original variables r, z by the function $l(r) = 200 - 0.05r$ for $0 \leq r \leq 3339$ m. The source, of frequency $f_0 = 25$ Hz, was placed at $z_s = 100$ m and modeled by the initial value $\psi_0(z) = \sqrt{\frac{k_0}{2}}\{\exp(-(z-z_s)^2\frac{k_0^2}{4}) - \exp(-(z+z_s)^2\frac{k_0^2}{4})\}$, $0 \leq z \leq l(0)$. The water was assumed to have constant sound speed equal to $c = c_0 = 1500$ m/sec and no attenuation. In (PN) $g_B(r)$ was taken equal to $\mathrm{i}k_0$. The problem was transformed by the change of variables (1.6) to an equivalent one on the horizontal strip $0 \leq x \leq 1$, $0 \leq t \leq T$, and it was solved numerically in both the $(\mathcal{N})$ and $(\mathcal{AK})$ formulations with $h = \frac{1}{1000}$, $k = \frac{T}{1000}$, and $T = 3339$. (In the figures that follow we present the numerical results after transforming them back to the original r, z variables. Specifically, we present graphs of the numerically computed field ψ, represented as is customary in underwater acoustics, by the transmission loss function TL$= -20\log_{10}(|\psi(z,r)|) + 10\log_{10} r$ dB depicted as a function of r at certain depths z.) For this upsloping example we show in Figure 1 the transmission loss curves as functions of $r \in [0, 2200 \text{ m}]$ at a depth of $z = 90$ m for both the $(\mathcal{N})$ and $(\mathcal{AK})$ models, which evidently agree very well.

We then considered the analogous downsloping wedge given by $l(r) = 33.05 + 0.05r$ for $0 \leq r \leq 3339$ m. The source, of frequency 25 Hz, was placed at $z_s = 25$ m and modeled as in the upsloping case. In this case, we found that the numerical solution of the problem $(\mathcal{N})$ apparently exhibited numerical instabilities and did not seem to converge as the discretization parameters became smaller. For example, in Figure 2 we superimpose (at depth $z = 25$ m and for ranges up to $T = 3339$) the TL curves corresponding to the $(\mathcal{N})$ model with $h = \frac{1}{100}$, $k = \frac{T}{100}$, and $h = \frac{1}{1000}$, $k = \frac{T}{1000}$, on the analogous results obtained by $(\mathcal{AK})$ with $h = \frac{1}{1000}$, $k = \frac{T}{1000}$. The $(\mathcal{AK})$ model yields reasonable results that converge to the solution shown with dotted line. To make sure that the numerical method used for $(\mathcal{N})$ was not the culprit, we repeated the numerical experiment using a Crank–Nicolson *finite difference* discretization for $(\mathcal{N})$ and found results identical to those of our finite element scheme. We tentatively conclude, therefore, that in this realistic downsloping bottom case, the model $(\mathcal{N})$ allows the growth of instabilities, in agreement with the remarks of Abrahamsson and Kreiss in [1] and [2].

To check the validity of the $(\mathcal{AK})$ solution of this problem, we compared the

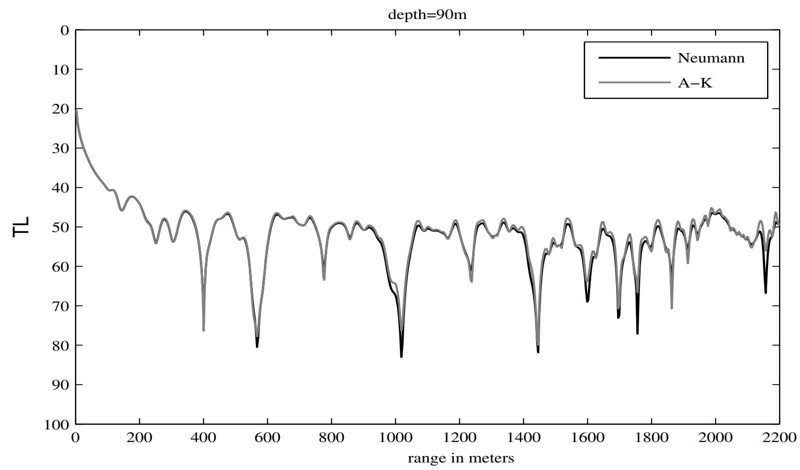

FIG. 1. *Upsloping ASA wedge; TL as a function of r at depth $z = 90$ m, comparison of ($\mathcal{N}$) and ($\mathcal{AK}$).*

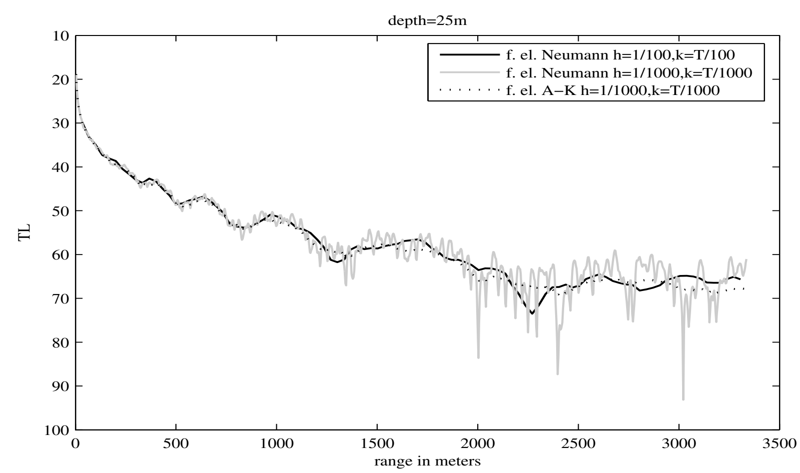

FIG. 2. *Downsloping ASA wedge;* TL *as a function of r at depth $z = 25$ m. (FE) solutions for the ($\mathcal{N}$) and ($\mathcal{AK}$) models.*

results of Figure 2 with those of yet another numerical method, the Crank–Nicolson type finite difference code IFD for the (PE) [17], [18], [19], which has been widely used in underwater acoustic numerical simulations. We chose the option of the rigid bottom boundary condition in IFD and solved the problem using $\Delta z = 3.31$ m, $\Delta r = 0.17$ m values by which the IFD solution had converged. (The IFD code solves the problem in the original r, z wedge-shaped domain.) The TL curves obtained at $z = 25$ m by ($\mathcal{AK}$) model solved numerically by the finite element scheme with $h = \frac{1}{1000}$, $k = \frac{T}{1000}$, $T = 3339$ (as in Figure 2) and for the IFD with the rigid bottom boundary condition agree practically within line thickness in a graph with the axes scaled as in Figure 2. In fact, they differ by about half a dB, as inspection of a typical window shown in Figure 3 reveals. (It is worthwhile to note that at a higher frequency $f_0 = 80$ Hz the

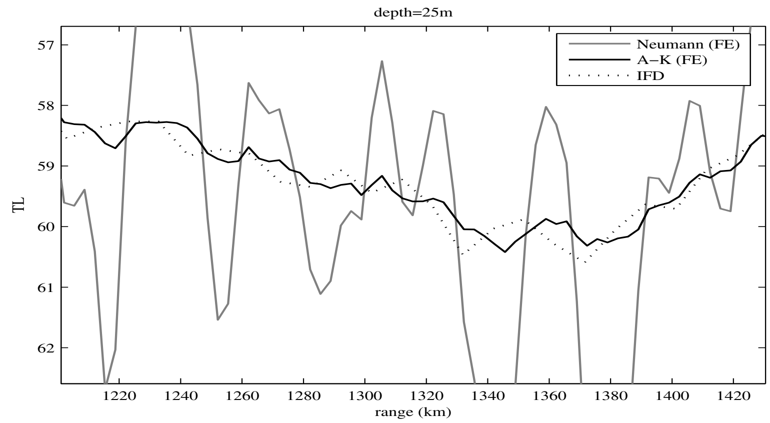

FIG. 3. *Downsloping ASA wedge; TL as a function of r at a depth $z = 25$ m. Comparison of $(\mathcal{N})$ and $(\mathcal{AK})$, discretized by (FE), and IFD with rigid bottom boundary conditions.*

results of $(\mathcal{N})$ approach those of $(\mathcal{AK})$ and IFD.)

To explain this result we looked closely at how IFD implements the rigid bottom boundary condition and found that it does not actually discretize (PN); instead, it uses a different boundary condition obtained by replacing the ψ_r term in (PN) by $\frac{\mathrm{i}}{2k_0}\psi_{zz} + \frac{\mathrm{i}k_0}{2}(\eta^2 - 1)\psi$ using the (PE), and then discretizing the ψ_{zz} term at the bottom with one-sided finite differences from the interior of the domain. In the next subsection we offer an explanation why this rigid bottom boundary condition yields a stable problem for any monotone bottom profile.

Our tentative conclusion, then, from this experiment is that in the case of realistic, downsloping environments, $(\mathcal{AK})$ and the rigid bottom boundary condition model implemented by IFD apparently yield correct results, while the Neumann bottom boundary condition used in $(\mathcal{N})$, which retains the term ψ_r at the bottom, allows the growth of instabilities.

3.2. Using the pde in the dynamical boundary condition. Let $w = w(t, y)$ be defined for $0 \le y \le s(t)$, $0 \le t \le T$, and satisfy (1.1)–(1.4). Replace the term $w_t(t, s(t))$ in (1.4) by its value given by the pde in (1.1) to obtain

$$w_y(t,s(t)) - \dot{s}(t)\left\{ \tfrac{\mathrm{i}}{2}\, w_{yy}(t,s(t)) + \left[\mathrm{i}\,\gamma(t,s(t)) + g(t)\right] w(t,s(t)) \right\} = 0 \quad \forall\, t \in [0,T]. \tag{3.1}$$

In the IFD code, the rigid bottom boundary condition used is a finite difference discretization of (3.1).

To avoid the presence of the second derivative $w_{yy}(t, s(t))$ in the boundary condition (3.1), we differentiate (1.1) with respect to y and put $\widetilde{p}(t, y) = w_y(t, y)$. (Note that $w(t, y) = \int_0^y \widetilde{p}(t, \xi)\, d\xi$ since $w(t, 0) = 0$.) Then, the ibvp (1.1)–(1.3), (3.1) becomes

$$\begin{aligned}
&\widetilde{p}_t = \tfrac{\mathrm{i}}{2}\,\widetilde{p}_{yy} + \mathrm{i}\,\gamma(t,y)\,\widetilde{p} + \mathrm{i}\,\gamma_y(t,y)\, w \quad \forall\, y \in [0,s(t)], \quad \forall\, t \in [0,T],\\
&\widetilde{p}_y(t,0) = 0 \quad \forall\, t \in [0,T],\\
&\widetilde{p}(t,s(t)) - \dot{s}(t)\left\{\tfrac{\mathrm{i}}{2}\,\widetilde{p}_y(t,s(t)) + \left[\,\mathrm{i}\,\gamma(t,s(t)) + g(t)\,\right] w(t,s(t))\right\} = 0 \quad \forall\, t \in [0,T],\\
&\widetilde{p}(0,y) = \widetilde{p}_0(y) := w_0'(y) \quad \forall\, y \in [0,s(0)].
\end{aligned} \tag{3.2}$$

(Note that using the (1.1) at $y = 0$ and the surface boundary condition $w(t, 0) = 0$, we obtain that $\widetilde{p}_y(t, 0) = w_{yy}(t, 0) = 0$.)

In what follows, we shall obtain an a priori L^2 bound for the solution of (3.2) and then propose a finite element method for solving it. With this aim in mind, we perform as usual the range-dependent change of depth variable $x := \frac{y}{s(t)}$ that maps the domain of the problem onto the horizontal strip $\{(t, x) : t \in [0, T],\, x \in \overline{D}\}$, where $D = (0, 1)$. Consider the transformation

$$\widetilde{p}(t, y) = \tfrac{1}{s(t)} \exp(-\zeta(t, x)) \left(p(t, x) - \zeta_x(t, x) \int_0^x p(t, \xi)\, d\xi \right), \tag{3.3}$$

where the function ζ will be specified below. After some calculations, we may derive the inverse of the transformation (3.3) in the form

$$p(t, x) = s(t) \exp(\zeta(t, x)) \left(\widetilde{p}(t, xs(t)) + \zeta_x(t, x) \int_0^x \widetilde{p}(t, \xi\, s(t))\, d\xi \right).$$

We also obtain that the function θ, defined by $\theta(t, x) := \int_0^x p(t, \xi) d\xi$ for $(t, x) \in [0, T] \times \overline{D}$, satisfies the relation

$$\theta(t, x) = \exp(\zeta(t, x))\, w(t, xs(t)), \quad (t, x) \in [0, T] \times \overline{D}. \tag{3.4}$$

Following the ideas of [4], and after analogous computations (see, in particular, (2.7) and (2.8) of [4]), we may deduce that p solves a well posed ibvp, in the case of strictly monotone bottoms, i.e., when $\dot{s}(t)$ is either positive or negative for all $t \in [0, T]$. To see this, define first ζ, as in [4], by the formula

$$\zeta(t, x) = \tfrac{\mathrm{i}}{2} (\sigma(t) - 1)\, \dot{s}(t)s(t)\, x^2 \quad \forall\, (t, x) \in [0, T] \times \overline{D}, \tag{3.5}$$

where $\sigma(t) := \frac{2(1+\dot{s}(t)^2)}{\dot{s}(t)^2} + \varepsilon$, if $\dot{s}(t) > 0$, where ε is a positive constant, and $\sigma(t) := 1$, or equivalently $\zeta = 0$, if $\dot{s}(t) < 0$. Then, in the transformed domain, the ibvp (3.2) becomes

$$\begin{aligned} & p_t = \tfrac{\mathrm{i}}{A(t)}\, p_{xx} + B(t, x)\, p_x \\ & \qquad\qquad + [\, B_x(t, x) + G(t, x)\,]\; p + G_x(t, x)\, \theta \;\; \forall\, (t, x) \in [0, T] \times \overline{D}, \\ & p_x(t, 0) = 0 \quad \forall\, t \in [0, T], \\ & \mathrm{i}\, \tfrac{1}{A(t)}\, p_x(t, 1) = \tfrac{1 - R_1(t)\, B(t,1)}{R_1(t)}\, p(t, 1) - \tfrac{R_1(t)\, G(t,1) + R_2(t)}{R_1(t)}\, \theta(t, 1) \quad \forall\, t \in [0, T], \\ & p(0, x) = p^0(x) \quad \forall\, x \in \overline{D}, \end{aligned} \tag{3.6}$$

where $p^0(x) = s(0) \exp(\zeta(0, x)) \left[w_0'(xs(0)) + \zeta_x(0, x) \int_0^x w_0'(\xi s(0))\, d\xi \right]$, $A(t) = 2\, s^2(t)$, $R_1(t) = \frac{\dot{s}(t)s(t)}{1+(\dot{s}(t))^2}$, $B(t, x) = x\, \frac{\dot{s}(t)}{s(t)} - \frac{\mathrm{i}}{s^2(t)}\, \zeta_x(t, x)$, $G(t, x) = \zeta_t(t, x) - x\, \frac{\dot{s}(t)}{s(t)}\, \zeta_x(t, x) + \mathrm{i}\, \gamma(t, xs(t)) + \frac{\mathrm{i}}{2s^2(t)} \left[(\zeta_x(t, x))^2 - \zeta_{xx}(t, x) \right]$, $R_2(t) = [\, g(t) - \zeta_t(t, 1)\,]\, R_1(t) + \zeta_x(t, 1)$. (Recall that $\theta(t, x) = \int_0^x p(t, \xi)\; d\xi$. In addition, note that (3.5) yields that B is real-valued and is given by $B(t, x) = x \frac{\dot{s}(t)}{s(t)}\, \sigma(t)$, so that $B(t, 0) = 0$ and $B_x(t, x) = B(t, 1) = \frac{\dot{s}(t)}{s(t)}\, \sigma(t)$. It is easily checked that $1 - R_1(t)\, B(t, 1) \neq 0$ for $t \in [0, T]$.)

We may now prove the following result.

THEOREM 3.1. *If the bottom is strictly monotone, the ibvp* (3.6) *is L^2-stable.*

Proof. Multiply the pde in (3.6) by $\overline{p(t,x)}$, integrate with respect to x in $[0,1]$, use integration by parts, and take real parts to obtain

$$\begin{aligned}\tfrac{1}{2}\tfrac{d}{dt}\|p(t,\cdot)\|^2 = \tfrac{2-R_1(t)\,B(t,1)}{2R_1(t)}\,|p(t,1)|^2 - \mathrm{Re}\Big[\tfrac{G(t,1)\,R_1(t)+R_2(t)}{R_1(t)}\,\theta(t,1)\,\overline{p(t,1)}\Big]\\ + \mathrm{Re}\big(G_x(t,\cdot)\,\theta(t,\cdot),p(t,\cdot)\big)\\ + \tfrac{1}{2}\big(B_x(t,\cdot)p(t,\cdot),p(t,\cdot)\big) + \mathrm{Re}\big(G(t,\cdot)\,p(t,\cdot),p(t,\cdot)\big)\quad \forall\, t\in[0,T].\end{aligned}$$

Using the Cauchy–Schwarz inequality, the arithmetic-geometric mean inequality, and noting that $|\theta(t,1)| \le \|p(t,\cdot)\|$, $\|\theta(t,\cdot)\| \le \|p(t,\cdot)\|$, we see from the above equation that for any $\xi > 0$ there exists a constant $C_\xi > 0$ such that

$$\tfrac{d}{dt}\|p(t,\cdot)\|^2 \le \Big(\tfrac{1}{R_1(t)} - \tfrac{1}{2}\,B(t,1) + \xi\Big)\,|p(t,1)|^2 + C_\xi\,\|p(t,\cdot)\|^2\quad \forall\, t\in[0,T].$$

Since $\frac{1}{R_1(t)} - \frac{1}{2}B(1,t) < 0$ for $t\in[0,T]$, we may chose ξ sufficiently small to make the first term in the right-hand side of the above negative. Hence, by Grönwall's lemma, we conclude that $\|p(t,\cdot)\| \le C\|p^0\|$ for $t\in[0,T]$, which ends the proof. ∎

Now, we can define a semidiscrete approximation $p_h : [0,T] \to S_h$ of the solution p of problem (3.6) by

$$p_h(0,x) = p_h^0(x)\quad \forall\, x\in\overline{D},$$

and

$$\begin{aligned}(\partial_t p_h,\phi) = -\tfrac{\mathrm{i}}{A(t)}\,\mathcal{B}(p_h,\phi) + \Big[\tfrac{1-R_1(1)B(t,1)}{R_1(t)}\,p_h(t,1) - \tfrac{R_1(t)G(1,t)+R_2(t)}{R_1(t)}\,\theta_h(t,1)\Big]\,\overline{\phi(1)}\\ + \big(B(t,\cdot)\,\partial_x p_h,\phi\big) + \big([B_x(t,\cdot)+G(t,\cdot)]p_h,\phi\big)\\ + \big(G_x(t,\cdot)\theta_h,\phi\big)\quad \forall\,\phi\in S_h,\quad \forall\, t\in[0,T],\end{aligned}$$

where $\theta_h(t,x) := \int_0^x p_h(t,\xi)\,d\xi$ and $p_h^0 \in S_h$ is a given reasonable approximation of p^0. Consequently, using (3.4), we see that $\exp(-\zeta(t,x))\theta_h(t,x)$ is an approximation of the solution $w(t,xs(t))$ of the ibvp (1.1)–(1.4). Also, it follows, as in Theorem 3.1, that there exists a positive constant C such that $\|p_h(t,\cdot)\| \le C\,\|p_h^0\|$ for $t\in[0,T]$.

3.3. Growth of solutions of ($\mathcal{N}$) for various bottom shapes. The final set of numerical experiments that we report concern the behavior of the size of the solutions of ($\mathcal{N}$), as t grows, in the presence of bottom profiles of various shapes. Recall that in [1] it was shown that ($\mathcal{N}$) is well posed if s is strictly monotone, i.e., if $\dot{s}(t) > 0$ or $\dot{s}(t) < 0$ for $t\in[0,T]$. In addition, downsloping bottom profiles were identified for which the solution of ($\mathcal{N}$) grew exponentially with t. (The fact that problems may arise in case $\dot{s}$ changes sign may be expected, in view of the analogous difficulties encountered in the (real) parabolic case; cf., e.g., [8].)

The ibvp ($\mathcal{N}$) was solved numerically up to $T = 1$, with $\beta = f = g = 0$, $u_0(x) = -x(x-1)^3$, $0 \le x \le 1$, with mesh parameters $h = k = \frac{1}{500}$, for eight bottom profiles $s(t)$, $0 \le t \le 1$, labeled (a) to (h) and shown in the left-hand icons of the pairs in Figure 4. (In all cases depth increases downwards.) The right-hand icon shows the corresponding, numerically computed L^2-norm of the solution of ($\mathcal{N}$) $\|u(t,\cdot)\|$ for $0 \le t \le 1$. (Note that $\|u(0,\cdot)\| = \frac{1}{6\sqrt{7}} \cong 0.062994$.) The bottom profiles

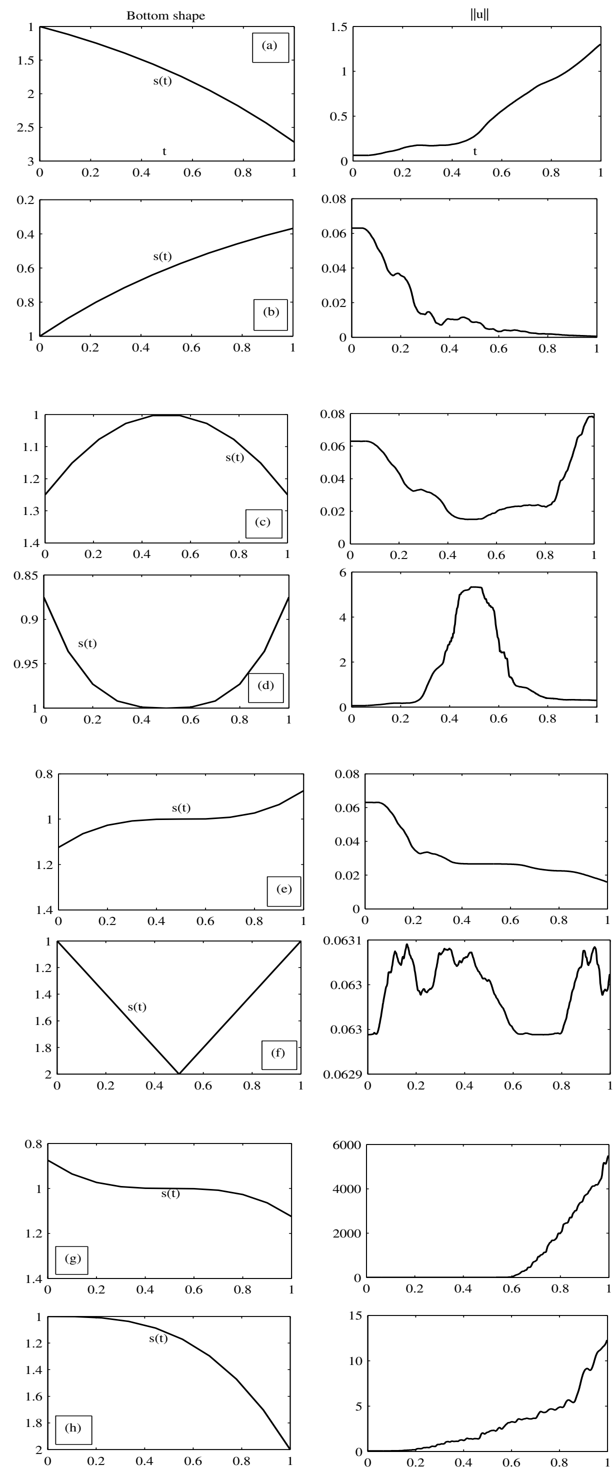

FIG. 4. *Behavior of the L^2-norm of the numerical solution of* $(\mathcal{N})$ *as function of* t *for bottom profiles* $s(t)$ *given by* (a)–(h).

are given for $0 \le t \le 1$ by the following expressions: (a) $s(t) = e^t$, (b) $s(t) = e^{-t}$, (c) $s(t) = 1 + (t - 0.5)^2$, (d) $s(t) = 1 - |t - 0.5|^3$, (e) $s(t) = 1 - (t - 0.5)^3$, (f) $s(t) = 2 - |2t - 1|$, (g) $s(t) = 1 + (t - 0.5)^3$, and (h) $s(t) = 1 + t^3$. Only (a) and (b) correspond to strictly monotone profiles for which the theory of [1] properly applies. In the cases (c), (d), (f) there is a change in monotonicity, in (e) and (g) we have that $\dot{s}(t) = \ddot{s}(t) = 0$ at $t = \frac{1}{2}$, while in (h) there holds that $\dot{s}(0) = \ddot{s}(0) = 0$. (In the case (f) a t-mesh node was placed at $t = 0.5$, where $\dot{s}$ fails to exist.)

We observe that the solution maintains a small L^2-norm in upsloping, like (b), or eventually upsloping bottoms, as in the cases of the trenches (d) and (f). There is a considerable growth of $\|u\|$ in the examples wherein the bottom profile is eventually downsloping; see (a), (c), (g), and (h) in agreement with the observations in [1], [2]. We note that in the case (g), an apparent singularity develops at $t = \frac{1}{2}$, where the bottom curvature changes sign (with horizontal tangent) and the bottom becomes downsloping. This apparently causes the L^2-norm to grow violently for $t > \frac{1}{2}$. A relatively weaker, but sizeable growth is also observed in (h), where the bottom is such that $\dot{s} = \ddot{s} = 0$ at $t = 0$ and is monotonically downsloping for $t > 0$. One cannot, of course, be certain about the existence of a singularity at $t = \frac{1}{2}$ in the case (g), given that the code does not at present possess an adaptive refinement capability in x and t. However, when the experiment was repeated with $k = h = \frac{1}{800}$, it was confirmed that the onset of rapid growth occurred at about $t = \frac{1}{2}$; for this mesh size, $\|u\|$ became of order $O(10^4)$ at $t = 1$.

4. A parabolic problem with a dynamical boundary condition.

Here we consider the model one-dimensional (real) parabolic problem (1.14) with a dynamical boundary condition analogous to that of $(\mathcal{N})$, which we rewrite here for ease in reading: We seek a real-valued function $u : [0, T] \times [0, 1] \to \mathbb{R}$, such that

$$
\begin{aligned}
&u_t = a(t)\, u_{xx} + \beta(t, x)\, u + f(t, x) \quad \forall\, (t, x) \in [0, T] \times [0, 1],\\
&u(t, 0) = 0 \quad \forall\, t \in [0, T],\\
&a(t)\, u_x(t, 1) = \varepsilon(t)\, u_t(t, 1) + \delta(t)\, u(t, 1) + g(t) \quad \forall\, t \in [0, T],\\
&u(x, 0) = u_0(x) \quad \forall\, x \in [0, 1],
\end{aligned}
\tag{4.1}
$$

where $\beta : [0, T] \times [0, 1] \to \mathbb{R}$, $f : [0, T] \times [0, 1] \to \mathbb{R}$, $\delta : [0, T] \to \mathbb{R}$, $g : [0, T] \to \mathbb{R}$, $a : [0, T] \to (0, +\infty)$ with $a_\star := \inf_{[0,T]} a > 0$, $\varepsilon : [0, T] \to \mathbb{R}$, $u_0 : [0, 1] \to \mathbb{R}$ are given smooth functions. We shall construct and analyze Galerkin-finite element approximations for the solution of (4.1), considering two different cases depending on the sign of ε.

4.1. The dissipative case.

The dissipative case is characterized by the assumption $\varepsilon(t) \le 0$ for $t \in [0, T]$; the problem is well posed; see, e.g., [15]. We assume that its solution is smooth enough for the purposes of the error estimates to follow. We adopt the notation and the assumptions of subsection 2.1, restricting ourselves to the real case, and avoiding the inverse inequality (2.5).

4.1.1. Semidiscrete approximation.

Find $u_h : [0, T] \to S_h$, a space-discrete approximation of u, requiring

$$
\begin{aligned}
(\partial_t u_h(t, \cdot), \chi) = {}& \big[\, \varepsilon(t)\, \partial_t u_h(t, 1) + \delta(t)\, u_h(t, 1) + g(t) \,\big]\, \chi(1) - a(t)\, \mathcal{B}(u_h(t, \cdot), \chi)\\
&+ (\beta(t, \cdot)\, u_h(t, \cdot), \chi) + (f(t, \cdot), \chi) \quad \forall\, \chi \in S_h, \quad \forall\, t \in [0, T],
\end{aligned}
\tag{4.2}
$$

and

$$u_h(0,\cdot) = R_h u_0(\cdot). \tag{4.3}$$

THEOREM 4.1. *Let $\varepsilon(t) \le 0$ for $t \in [0,T]$. Then, the problem (4.2)–(4.3) has a unique solution $u_h \in C^1([0,T];S_h)$. If u is the solution of (4.1), we have for $h \in (0,h_\star]$ and $t \in [0,T]$*

$$\|u_h(t,\cdot) - R_h u(t,\cdot)\|_1^2 \le C\, h^{2(r+1)} \left(\int_0^t \Gamma_D(\tau)\, d\tau \right), \tag{4.4}$$

and

$$\begin{aligned} &\|u_h(t,\cdot) - u(t,\cdot)\| + h\,\|u_h(t,\cdot) - u(t,\cdot)\|_1 \\ &\qquad \le C\, h^{r+1} \left[\|u(t,\cdot)\|_{r+1} + \left(\int_0^t \Gamma_D(\tau)\, d\tau \right)^{\frac{1}{2}} \right], \end{aligned} \tag{4.5}$$

where $\Gamma_D(\tau) := \|u(\tau,\cdot)\|_{r+1}^2 + \|\partial_t u(\tau,\cdot)\|_{r+1}^2$.

Proof. The existence and uniqueness of $u_h \in C^1([0,T];S_h)$ follows if we argue as in Proposition 2.3. Let $h \in (0,h_\star]$ and $\theta_h := u_h - R_h u$. Using (4.2), the pde in (4.1), (2.6), and (2.8), we obtain

$$\begin{aligned} (\partial_t \theta_h(t,\cdot), \chi) = {}& \big[\, \varepsilon(t)\, \partial_t \theta_h(t,1) + \delta(t)\, \theta_h(t,1) \,\big]\, \chi(1) - a(t)\, \mathcal{B}(\theta_h(t,\cdot), \chi) \\ & + (\beta(t,\cdot)\, \theta_h(t,\cdot), \chi) + \big(\Phi_\star(t,\cdot), \chi \big) \quad \forall\, \chi \in S_h, \quad \forall\, t \in [0,T], \end{aligned} \tag{4.6}$$

where $\Phi_\star := [\partial_t u - R_h(\partial_t u)] - \beta\,(u - R_h u)$. First we observe that from (2.7) it follows that

$$\|\Phi_\star(t,\cdot)\| \le C\, h^{r+1} \big[\, \|u(t,\cdot)\|_{r+1} + \|\partial_t u(t,\cdot)\|_{r+1} \,\big] \quad \forall\, t \in [0,T]. \tag{4.7}$$

Setting $\chi = \theta_h$ in (4.6) and using (2.3) and (4.7), we get

$$\epsilon\, \tfrac{d}{dt} \|\theta_h(t,\cdot)\|^2 \le |\varepsilon(t)|\, |\partial_t \theta_h(t,1)|^2 + C\, (\epsilon + \epsilon^3)\, \|\theta_h(t,\cdot)\|^2 + \epsilon\, h^{2(r+1)}\, \Gamma_D(t) \tag{4.8}$$

for all $t \in [0,T]$ and $\epsilon > 0$.

In addition, for $\chi = \partial_t \theta_h$ in (4.6) and in view of (2.3) and (4.7) we get

$$\begin{aligned} \tfrac{d}{dt} \big[\, a(t)\, |\theta_h(t,\cdot)|_1^2 - \delta(t)\, |\theta_h(t,1)|^2 \,\big] \le {}& -2\, |\varepsilon(t)|\, |\partial_t \theta_h(t,1)|^2 \\ & + C\, \|\theta_h(t,\cdot)\|_1^2 + h^{2(r+1)}\, \Gamma_D(t) \end{aligned} \tag{4.9}$$

for all $t \in [0,T]$. For positive ϵ we define

$$\nu_\epsilon(t) := \epsilon\, \|\theta_h(t,\cdot)\|^2 + a(t)\, |\theta_h(t,\cdot)|_1^2 - \delta(t)\, |\theta_h(t,1)|^2 \quad \forall\, t \in [0,T]. \tag{4.10}$$

Then, applying the trace inequality (2.3), we have

$$\begin{aligned} \nu_\epsilon(t) &\ge \epsilon\, \|\theta_h(t,\cdot)\|^2 + a_\star\, |\theta_h(t,\cdot)|_1^2 - 2|\delta(t)|\, \|\theta_h(t,\cdot)\|\, |\theta_h(t,\cdot)|_1 \\ &\ge \tfrac{a_\star}{2}\, |\theta_h(t,\cdot)|_1^2 + \left(\epsilon - \tfrac{2\,|\delta(t)|^2}{a_\star} \right) \|\theta_h(t,\cdot)\|^2 \quad \forall\, t \in [0,T]. \end{aligned} \tag{4.11}$$

If $\epsilon_0 := \frac{a_\star}{2} + \frac{2}{a_\star} \max_{[0,T]} |\delta|^2$, (4.11) yields that

$$\nu_{\epsilon_0}(t) \geq \tfrac{a_\star}{2} \|\theta_h(t,\cdot)\|_1^2 \quad \forall\, t \in [0,T]. \tag{4.12}$$

Now, setting $\epsilon = \epsilon_0$ in (4.8) and then adding the resulting equation with (4.9), we obtain

$$\tfrac{d}{dt}\nu_{\epsilon_0}(t) \leq C\,\nu_{\epsilon_0}(t) + (\epsilon_0 + 1)\, h^{2(r+1)}\, \Gamma_D(t) \quad \forall\, t \in [0,T]. \tag{4.13}$$

Since $\theta_h(0,\cdot) = 0$, the bound (4.4) follows from (4.13) via Grönwall's lemma and (4.12). The error estimate (4.5) follows in view of (2.7). ∎

4.1.2. Crank–Nicolson fully discrete approximations. We use the notation of subsection 2.2.2. For $n = 0, \dots, N$, the Crank–Nicolson method for the problem (4.1) yields an approximation $U_h^n \in S_h$ of $u(t^n,\cdot)$ as follows:

Step 1. Set

$$U_h^0 := R_h u_0. \tag{4.14}$$

Step 2. For $n = 1, \dots, N$, find $U_h^n \in S_h$ such that

$$\begin{aligned}(\partial U_h^n, \chi) = {} & \Big[\, \varepsilon^{n-\frac12}\, \partial U_h^n(1) + \delta^{n-\frac12}\, \mathcal{A}U_h^n(1) + g^{n-\frac12} \,\Big]\, \chi(1) \\ & - a^{n-\frac12}\, \mathcal{B}\big(\mathcal{A}U_h^n, \chi\big) + \big(\beta^{n-\frac12}\, \mathcal{A}U_h^n, \chi\big) + \big(f^{n-\frac12}, \chi\big) \quad \forall\, \chi \in S_h,\end{aligned} \tag{4.15}$$

where $a^{n-\frac12} := a(t^{n-\frac12})$, $\delta^{n-\frac12} := \delta(t^{n-\frac12})$, $\varepsilon^{n-\frac12} := \varepsilon(t^{n-\frac12})$, $g^{n-\frac12} := g(t^{n-\frac12})$, $f^{n-\frac12} := f(t^{n-\frac12},\cdot)$, and $\beta^{n-\frac12} := \beta(t^{n-\frac12},\cdot)$.

The following existence and consistency results are analogous to those of Propositions 2.5 and 2.6, and their proof is straightforward.

Proposition 4.2. *Let $n \in \{1, \dots, N\}$, and suppose that $U_h^{n-1} \in S_h$ is well defined. If $\varepsilon^{n-\frac12} \leq 0$, then there exists a constant C such that if $k_n < C$, then U_h^n is well defined by* (4.15).

Proposition 4.3. *Let u be the solution of* (4.1). *For $n = 1, \dots, N$, define $\sigma^n : \overline{D} \to \mathbb{R}$ by $\frac{u^n - u^{n-1}}{k_n} = a^{n-\frac12}\, u_{xx}(t^{n-\frac12},\cdot) + \beta^{n-\frac12}\, \mathcal{A}u^n + f^{n-\frac12} + \sigma^n$. Then*

$$\|\sigma^n\| \leq C\,(k_n)^2 \,\Big(\max_{[t^{n-1},t^n]} \|\partial_t^2 u\| + \max_{[t^{n-1},t^n]} \|\partial_t^3 u\|\Big), \quad n = 1, \dots, N.$$

The main result of this subsection is contained in the following theorem, which is stated here without proof. Its proof follows the general line of Theorem 2.7 and may be found in [6].

Theorem 4.4. *Let u be the solution of* (4.1), *and let $(U_h^n)_{n=0}^N$ be the fully discrete approximations that the method* (4.14)–(4.15) *produces. Assume that $\varepsilon(t) \leq 0$ for $t \in [0,T]$, and that* (2.28) *holds. Then, there exists a constant $C_D \geq 0$ such that if $\max_{1 \leq n \leq N}(k_n\, C_D) \leq \frac13$, there exists a constant $C > 0$ such that*

$$\max_{1 \leq n \leq N} \|U_h^n - R_h u^n\|_1 \leq C\,(k^2 + h^{r+1})\, \Upsilon_D(u) \quad \forall\, h \in (0, h_\star],$$

$$\max_{0 \leq n \leq N} \|U_h^n - u^n\|_\ell \leq C\,(k^2 + h^{r+1-\ell})\, \Upsilon_D(u) \quad \forall\, h \in (0, h_\star], \quad \ell = 0, 1,$$

where $\Upsilon_D(u) := \sum_{\ell=0}^{1} \max_{[0,T]} \|\partial_t^\ell u\|_{r+1} + \sum_{\ell=2}^{3} \max_{[0,T]} \|\partial_t^\ell u\|_1 + \sum_{\ell=2}^{4} \max_{t \in [0,T]} |\partial_t^\ell u(t,1)|$.

4.2. The reactive case. In this subsection, we propose and analyze finite element approximations in case the dynamical boundary condition in (4.1) is of reactive type, i.e., $\varepsilon(t) > 0$ for $t \in [0, T]$. According to [25], [9], the problem is well posed only in the one-dimensional case. To construct a finite element method we replace (cf. subsection 3.2) the term u_t in the dynamical boundary condition using the partial differential equation in (4.1). Hence we obtain $a(t)\, u_{xx}(t, 1) = \frac{a(t)}{\varepsilon(t)} u_x(1, t) - \left[\frac{\delta(t)}{\varepsilon(t)} + \beta(t, 1)\right] u(t, 1) - \left[\frac{g(t)}{\varepsilon(t)} + f(t, 1)\right]$ for $t \in [0, T]$. Then, to use this as a boundary condition, we formulate a variational formulation using $\mathcal{B}(\cdot, \cdot)$ instead of the $L^2(D)$ inner product $(\cdot, \cdot)$. Of course, this approach also works if $\varepsilon(t) < 0$ for $t \in [0, T]$.

4.2.1. Preliminaries. Let $r \in \mathbb{N}$ with $r \geq 3$, and $\mathcal{S}_h$ be a finite-dimensional subspace of $\mathbb{H}^2(D)$ consisting of C^1 functions that are polynomials of degree less or equal to r in each interval of a nonuniform partition of D with maximum length $h \in (0, h_\star]$. It is well known [10] that the following approximation property holds:

$$\inf_{\chi \in \mathcal{S}_h} \|v - \chi\|_2 \leq C\, h^{s-1}\, \|v\|_{s+1} \quad \forall\, v \in \mathbb{H}^{s+1}(D), \quad s = 1, \ldots, r, \quad \forall\, h \in (0, h_\star]. \tag{4.16}$$

We introduce bilinear forms $\mathcal{B}^\star$, $\gamma^\star : H^2(D) \times H^2(D) \to \mathbb{R}$ given by $\mathcal{B}^\star(v, w) := (v'', w'')$ and $\gamma^\star(v, w) := (v'', w'') + (v', w')$ for v and $w \in H^2(D)$, and set $|v|_2 := \|v''\|$ for $v \in H^2(D)$. Also, we define a new elliptic projection $R_h^\star : H^2(D) \to \mathcal{S}_h$ by

$$\gamma^\star(R_h^\star v, w) = \gamma^\star(v, \chi) \quad \forall\, \chi \in \mathcal{S}_h. \tag{4.17}$$

LEMMA 4.5. *The elliptic projection $R_h^\star$ has the following property:*

$$(R_h^\star v)'(1) = v'(1) + (R_h^\star v - v)(1) - \tfrac{1}{6}\, \mathcal{B}(R_h^\star v - v, \omega) \quad \forall\, v \in \mathbb{H}^2(D), \tag{4.18}$$

where $\omega(x) = x^3$.

Proof. Let $v \in \mathbb{H}^2(D)$ and $\rho = R_h^\star v - v$. Since $\omega \in \mathcal{S}_h$, setting $\chi = \omega$ in (4.17) we obtain $\int_D \rho''(x)\, x \; dx = -\frac{1}{6}\, (\rho', \omega')$. Then, integrating by parts we get $\rho'(1) = \rho(1) - \rho(0) - \frac{1}{6}\, (\rho', \omega')$, which is the desired equality, since $\rho(0) = 0$. ∎

PROPOSITION 4.6. *The elliptic projection $R_h^\star$ has the following approximation properties:*

$$\|R_h^\star v - v\|_1 + h\, \|R_h^\star v - v\|_2 \leq C\, h^s\, \|v\|_{s+1} \tag{4.19}$$

and

$$|(R_h^\star v - v)'(1)| + |(R_h^\star v - v)(1)| \leq C\, h^s\, \|v\|_{s+1} \tag{4.20}$$

for $s = 1, \ldots, r$, $v \in \mathbb{H}^{s+1}(D)$, and $h \in (0, h_\star]$.

Proof. Let $h \in (0, h_\star]$, $s \in \{1, \ldots, r\}$, $v \in \mathbb{H}^{s+1}(D)$, and $e = R_h^\star v - v$. Using (4.17), we have $\gamma^\star(e, e) = \gamma^\star(e, \chi - v)$ for $\chi \in \mathcal{S}_h$, which along with (4.16) yields

$$|e|_2 + |e|_1 \leq C\, h^{s-1}\, \|v\|_{s+1}. \tag{4.21}$$

Now, let $w \in H^3(D)$ such that

$$\begin{gathered} -w''' + w' = e' \quad \text{in} \quad D, \\ w(0) = w''(1) = w''(0) = 0. \end{gathered} \tag{4.22}$$

It is easily seen that (4.22) conceals a standard two-point boundary-value problem with respect to w' and thus existence and uniqueness of its solution follows in a straightforward way; in addition we have that $\|w\|_3 \le C\,|e|_1$. Thus, we obtain $\|e'\|^2 = \gamma^\star(e, w-\chi)$ for $\chi \in \mathcal{S}_h$. Then, we use (4.21) and (4.22) to get

$$\begin{aligned}|e|_1^2 &\le C\,\left(|e|_2 + |e|_1\right)\,h\,\|w\|_3\\ &\le C\,h^s\,\|v\|_{s+1}\,|e|_1,\end{aligned}$$

which yields $|e|_1 \le C\,h^s\,\|v\|_{s+1}$. Hence, (4.19) follows in view of (4.21). In addition, using (4.18), (2.3), (2.1), and (4.19) we have

$$\begin{aligned}|e'(1)|^2 + |e(1)|^2 &\le C\,\left(\,|e(1)|^2 + \|e'\|^2\,\right)\\ &\le C\,|e|_1^2\\ &\le C\,h^{2s}\,\|v\|_{s+1}^2,\end{aligned}$$

which obviously yields (4.20). ◻

For later use, we close this section by extending (2.3) as follows.

Lemma 4.7. *For $v \in H^2(D)$ it holds that*

$$|v'(1)|^2 \le |v|_1^2 + 2\,|v|_1\,|v|_2. \tag{4.23}$$

Proof. Let $v \in H^2(D)$. Observing that $|v'(1)|^2 = \int_D [(v'(x))^2\,x]'\,dx$, we obtain $|v'(1)|^2 = \|v'\|^2 + 2\int_D x\,v'(x)\,v''(x)\,dx$, which yields (4.23) via the Cauchy–Schwarz inequality. ◻

4.2.2. Semidiscrete approximation. We define $u_h : [0,T] \to \mathcal{S}_h$, a space-discrete approximation of u, requiring

$$\begin{aligned}\mathcal{B}(\partial_t u_h(t,\cdot),\chi) = \Big\{\, &\tfrac{a(t)}{\varepsilon(t)}\,\partial_x u_h(t,1) - \Big[\,\tfrac{\delta(t)}{\varepsilon(t)} + \beta(t,1)\Big]\,u_h(t,1)\\ &- \Big[\,\tfrac{g(t)}{\varepsilon(t)} + f(t,1)\Big]\,\Big\}\,\chi'(1) + f(t,0)\,\chi'(0)\\ &- a(t)\,\mathcal{B}^\star(u_h(t,\cdot),\chi) + \mathcal{B}(\beta(t,\cdot)\,u_h(t,\cdot),\chi)\\ &+ \mathcal{B}(f(t,\cdot),\chi)\quad \forall\,\chi \in \mathcal{S}_h,\quad \forall\,t\in[0,T],\end{aligned} \tag{4.24}$$

and

$$u_h(0,\cdot) = R_h^\star u_0(\cdot). \tag{4.25}$$

Theorem 4.8. *Let $\varepsilon(t) > 0$ for $t \in [0,T]$. Then the problem (4.24)–(4.25) has a unique solution $u_h \in C^1([0,T];\mathcal{S}_h)$. If u is the solution of (4.1) and Γ_D is the function specified in Theorem 4.1, we have*

$$\|u_h(t,\cdot) - u(t,\cdot)\|_1 \le C\,h^r\,\left[\|u(t,\cdot)\|_{r+1} + \left(\int_0^t \Gamma_D(\tau)\,d\tau\right)^{\frac{1}{2}}\right] \tag{4.26}$$

for all $t \in [0,T]$ and $h \in (0,h_\star]$.

Proof. Let $h \in (0, h_\star]$. The existence-uniqueness of u_h follows as in Proposition 2.3. Also, let $\theta_h := u_h - R_h^\star u$ and $\eta = R_h^\star u - u$. Using (4.24), (4.17), and (4.1), we obtain

$$\begin{aligned}\mathcal{B}(\partial_t \theta_h(t,\cdot),\chi) = \Big\{ &\tfrac{a(t)}{\varepsilon(t)}\,\partial_x\theta_h(t,1) - \Big[\tfrac{\delta(t)}{\varepsilon(t)} + \beta(t,1)\Big]\,\theta_h(t,1) + \mathcal{E}_{R,2}(t)\Big\}\,\chi'(1)\\ &- a(t)\,\mathcal{B}^\star(\theta_h(t,\cdot),\chi) + \mathcal{B}(\beta(t,\cdot)\,\theta_h(t,\cdot),\chi)\\ &+ \mathcal{B}\big(\mathcal{E}_{R,1}(t,\cdot),\chi\big)\\ &+ a(t)\,\mathcal{B}(R_h^\star u(t,\cdot) - u(t,\cdot),\chi) \quad \forall\,\chi \in \mathcal{S}_h, \quad \forall\, t \in [0,T],\end{aligned} \tag{4.27}$$

where

$$\mathcal{E}_{R,1} := [\partial_t u - R_h^\star(\partial_t u)] - \beta\,(u - R_h^\star u),$$

$$\mathcal{E}_{R,2}(t) := \tfrac{a(t)}{\varepsilon(t)}\,\partial_x\eta(t,1) - \Big[\tfrac{\delta(t)}{\varepsilon(t)} + \beta(t,1)\Big]\,\eta(t,1).$$

First, observe that using (4.19), (4.20), and (2.1), it follows that

$$|\,\mathcal{B}(\mathcal{E}_{R,1}(t,\cdot),\chi) + a(t)\,\mathcal{B}(\eta(t,\cdot),\chi)\,| \le C\,h^r\,\big(\,\|u(t,\cdot)\|_{r+1} + \|\partial_t u(t,\cdot)\|_{r+1}\,\big)\,|\chi|_1 \tag{4.28}$$

and

$$|\mathcal{E}_{R,2}(t)\,\chi'(1)| \le C\,h^r\,\|u(t,\cdot)\|_{r+1}\,|\chi'(1)| \tag{4.29}$$

for $\chi \in \mathcal{S}_h$ and $t \in [0,T]$. Then, set $\chi = \theta_h$ in (4.27) and use the Cauchy–Schwarz inequality, (2.1), (4.28), (4.29), (4.23), and (2.3) to get

$$\tfrac{1}{2}\,\tfrac{d}{dt}|\theta_h(t,\cdot)|_1^2 \le -a_\star\,|\theta_h(t,\cdot)|_2^2 + C\Big[\,|\theta_h(t,\cdot)|_1^2 + h^{2r}\,\Gamma_D(t) + |\theta_h(t,\cdot)|_1\,|\theta_h(t,\cdot)|_2\,\Big]$$

for all $t \in [0,T]$, which, along the arithmetic-geometric mean inequality, yields

$$\tfrac{d}{dt}|\theta_h(t,\cdot)|_1^2 \le C\,\big[\,|\theta_h(t,\cdot)|_1^2 + h^{2r}\,\Gamma_D(t)\,\big] \quad \forall\, t \in [0,T].$$

Since $\theta_h(0,\cdot) = 0$, using Grönwall's lemma we see that

$$|\theta_h(t,\cdot)|_1^2 \le C\,h^{2r}\left(\int_0^t \Gamma_D(\tau)\,d\tau\right) \quad \forall\, t \in [0,T]. \tag{4.30}$$

Finally, we combine (2.1), (4.30), and (4.19) to arrive at the error estimate (4.26). ◻

4.2.3. Crank–Nicolson fully discrete approximations. For $n = 0, \dots, N$, the Crank–Nicolson method for the problem (4.1) yields an approximation $U_h^n \in \mathcal{S}_h$ of $u(t^n,\cdot)$ as follows:

Step 1. Set

$$U_h^0 := R_h^\star u_0. \tag{4.31}$$

Step 2. For $n = 1, \ldots, N$, find $U_h^n \in \mathcal{S}_h$ such that

$$\begin{aligned}\mathcal{B}(\partial U_h^n, \chi) = \Bigg\{ & \frac{a^{n-\frac{1}{2}}}{\varepsilon^{n-\frac{1}{2}}} \, (\mathcal{A}U_h^n)'(1) - \left[\frac{\delta^{n-\frac{1}{2}}}{\varepsilon^{n-\frac{1}{2}}} + \beta^{n-\frac{1}{2}}(1) \right] \mathcal{A}U_h^n(1) \\ & - \left[\frac{g^{n-\frac{1}{2}}}{\varepsilon^{n-\frac{1}{2}}} + f^{n-\frac{1}{2}}(1) \right] \Bigg\} \, \chi'(1) + f^{n-\frac{1}{2}}(0) \, \chi'(0) \\ & - a^{n-\frac{1}{2}} \, \mathcal{B}^\star\big(\mathcal{A}U_h^n, \chi\big) + \mathcal{B}\big(\beta^{n-\frac{1}{2}} \, \mathcal{A}U_h^n, \chi\big) \\ & + \mathcal{B}\big(f^{n-\frac{1}{2}}, \chi\big) \quad \forall \, \chi \in \mathcal{S}_h.\end{aligned} \tag{4.32}$$

The proof of the following error estimate for the fully discrete approximation may be found in [6].

THEOREM 4.9. *Let $\varepsilon(t) > 0$ for $t \in [0, T]$. Then, there exists a constant C such that if $\max_{1 \le n \le N} k_n < C$, then $(U_h^n)_{n=1}^N$ are well defined by (4.31)–(4.32). In addition, if u is the solution of (4.1), there exists a constant $C_R \ge 0$ such that if $\max_{1 \le n \le N}(k_n \, C_R) \le \frac{1}{3}$, there exists a constant $C > 0$ such that*

$$\max_{1 \le n \le N} \|U_h^n - u^n\|_1 \le C \, (k^2 + h^r) \; \Upsilon_R(u) \quad \forall \, h \in (0, h_\star],$$

where

$$\Upsilon_R(u) := \sum_{\ell=0}^{1} \left[\max_{[0,T]} \|\partial_t^\ell u\|_{r+1} + \max_{t \in [0,T]} |\partial_t^2 \partial_x^\ell u(t, 1)| \right] + \sum_{\ell=2}^{3} \max_{[0,T]} |\partial_t^\ell u|_1 + \max_{[0,T]} |\partial_t^2 u|_2.$$

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