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.

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 modelled 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

$$(HE) \quad \Delta p + k_0^2 \eta^2(r,z)p = 0.$$ 

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 $z = 0$ and the range-dependent bottom $z = \ell(r)$ (see Fig. 1); $\ell = \ell(r)$ 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. (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

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

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

$$(N) \quad p_z - \ell'(r)p_r = 0 \quad \text{at} \quad z = \ell(r).$$
Applying the change of variables \( p(r, z) = \psi(r, z) \frac{1}{2k_0} \), assuming that \( 2ik_0|\psi_r| >> |\psi_{rr}| \) (narrow-angle paraxial approximation) and neglecting terms of \( O(\frac{1}{r}) \) (far-field approximation) we arrive (cf., e.g., [22], [18], [6]) at the standard ‘Parabolic’ Equation (PE), which is a linear Schrödinger equation of the form

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

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 \( 0 \leq z \leq \ell(r), \ r \geq 0 \). The (PE) will be supplemented by an initial condition \( \psi(0, z) = \psi_0(z), \ 0 \leq z \leq \ell(0) \), modelling the source at \( r = 0 \), the surface boundary condition \( \psi = 0 \) for \( z = 0, \ r \geq 0 \), and a bottom boundary condition obtained by transforming (D) or (N). The Dirichlet boundary condition (D) remains of the same type \( (\psi = 0 \text{ at } z = \ell(r)) \) while the Neumann boundary condition (N) is transformed to a condition of the form

\[
(\text{PN}) \quad \psi_z - \frac{\ell}{\ell(r)} \psi_r - g_\delta(r) \frac{\ell}{\ell(r)} \psi = 0 \quad \text{at} \quad z = \ell(r),
\]

where \( g_\delta(r) \) is complex-valued and is usually taken simply as \( i k_0 \).

The theory and numerical analysis of this initial-boundary-value problem (ibvp) with the Dirichlet bottom boundary condition is standard, cf. e.g. [19], [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 \( \ell(r) \) is not the zero function, due to the presence of the term \( \psi_r \) in (PN). In [1] Abrahamsson and Kreiss proved existence and uniqueness of solutions, in the case of a strictly monotone bottom, i.e. when \( \ell(r) \) is of one sign for \( r \geq 0 \).

![Figure 1. The domain of the initial boundary value problems for the (PE) in the \( r, z \) variables](image)

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

\[
(1.1) \quad w_t = \frac{1}{2} w_{yy} + i \gamma(t, y) w, \quad 0 \leq y \leq s(t), \quad t \geq 0.
\]

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

\[
(1.2) \quad w(0, y) = w_0(y) := \frac{1}{\psi_{\text{ref}}} \psi_0 \left( \frac{y}{s(t)} \right), \quad 0 \leq y \leq s(0).
\]

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

\[
(1.3) \quad w(t, 0) = 0, \quad t \geq 0,
\]

while the boundary condition (PN) becomes

\[
(1.4) \quad w_y(t, s(t)) - \dot{s}(t) \left[ w_t(t, s(t)) + g(t) w(t, s(t)) \right] = 0, \quad t \geq 0.
\]

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

\[
(1.5) \quad u(t, x) = \exp(-i \dot{s}(t)x^2) w(t, s(t)x),
\]
which defines the new field variable \( u(t, x) \) for \( 0 \leq x \leq 1, t \geq 0 \). In \( 1.5 \) \( \delta(t) := \frac{\dot{s}(t)s(t)}{1 + \dot{s}(t)^2}, \) \( t \geq 0, \) where a dot denotes differentiation with respect to \( t \). In terms of the new variables \( \ell \) becomes

\[
1.6 \quad u_t = i a(t) u_{xx} + i \beta(t, x) u, \quad 0 \leq x \leq 1, \quad t \geq 0,
\]

where, for \( 0 \leq x \leq 1, t \geq 0, \)

\[
\begin{align*}
a(t) &= \frac{1}{2s(t)}, & \beta(t, x) &= \beta_\mu(t, x) + i \beta_\nu(t, x), \\
\beta_\mu(t, x) &= \text{Re}[\gamma(t, xs(t))] - \frac{\dot{s}(t)s(t)^2}{2}, & \beta_\nu(t, x) &= \text{Im}[\gamma(t, xs(t))] + \frac{\dot{s}(t)}{2s(t)}.
\end{align*}
\]

The purpose of introducing in \( 1.6 \) the factor \( e^{-i\dot{s}(t)x^2} \) with \( \delta = \frac{i}{2} \) 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 \( 1.6, \) the initial and boundary conditions \( 1.7-1.9 \) change accordingly. Specifically, we have

\[
1.8 \quad u(0, x) = u_0(x) := e^{-i\dot{s}(0)x^2} u_0(xs(0)) \quad \forall x \in [0, 1],
\]

\[
1.9 \quad u(t, 0) = 0, \quad t \geq 0,
\]

and

\[
1.10 \quad u_x(t, 1) = s_1(t) u_t(t, 1) + m(t) u(t, 1), \quad t \geq 0,
\]

where

\[
1.11 \quad s_1(t) := \frac{\dot{s}(t)s(t)}{1 + \dot{s}(t)^2}, \quad m(t) := g(t)s_1(t) + i(s_1(t)\dot{s}(t) - 2\delta(t)), \quad t \geq 0.
\]

The boundary condition \( 1.10 \) is an example of a dynamical boundary condition, because it involves (if \( \dot{s} \neq 0 \)) the value of \( u_x \) 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 \( \dot{s}(t) \leq 0 \), and that the problem has a unique solution, smooth enough for the purposes of the error estimation. In paragraphs 2.1 and 2.2 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 \( u_x \) term in \( 1.10 \): the condition \( \dot{s}(t) \leq 0 \), which implies that \( s_1(t) \leq 0 \), is needed to obtain a basic energy inequality for the error of the semidiscretization). Subsequently, in paragraph 2.2, we discretize the semidiscrete problem in \( t \) variable using a Crank-Nicolson type method with a variable step-length. Again, under the assumption that \( \dot{s}(t) \leq 0 \) for \( 0 \leq t \leq T \), 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 \( \text{PE} \), is of the form

\[
1.12 \quad \psi_z - i k_0 \ell(r) \psi = 0 \quad \text{at} \quad z = \ell(r).
\]

This condition may be viewed as a ‘paraxialization’ of (PN). When the nondimensionalization \( z \rightarrow y, r \rightarrow t, \psi \rightarrow w \) is performed, (AK) becomes

\[
1.13 \quad w_y(t, s(t)) - i \dot{s}(t) w(t, s(t)) = 0, \quad t \geq 0.
\]

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

\[
1.14 \quad u_x(t, 1) = 0, \quad t \geq 0.
\]

The proof of the well-posedness of the ibvp consisting of \( \{1.6-1.9\} \) and \( 1.13 \) is standard, cf. \( 19 \). Its numerical analysis too is straightforward; under no restriction on the sign of \( \dot{s}(t) \) we prove in paragraph 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. As predicted by the theoretical stability and convergence analysis, the finite element scheme is stable and second-order accurate when Neumann boundary conditions are considered in domains with upsloping bottoms. (It also appears to be convergent in small scale problems with downsloping bottoms and also in more realistic examples if the downsloping bottom has very small slope.) The scheme with the Abrahamsson-Kreiss condition behaved well, as predicted by the theory, in all examples of bottoms of arbitrary shape that we ran.

When we compared the results of the schemes using both boundary conditions in the case of the upsloping and downsloping rigid bottom ASA wedge (a standard test problem for long range sound propagation in underwater acoustics, [15]), we 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, [16, 17, 18], implemented with the rigid bottom boundary condition option. The IFD scheme uses a discretized version of the Neumann boundary condition (PN), wherein the \( \psi \) 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 [21] 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 [21] is similar to the one analyzed here in the case of the Abrahamsson-Kreiss bottom boundary condition. We have considerably modified the analysis of [21] and obtain optimal-order estimates, since, by using the transformation (1.9), 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 [4].

The problem addressed in the present paper, namely sound propagation modelled 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 modelled by the (PE) in each layer with transmission conditions (continuity of \( \psi \) and of \( \frac{1}{\rho} \frac{\partial \omega}{\partial n} \), where \( \rho \) 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 \( \psi_r \) 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 non-homotheticity of the layers has to be balanced by the jump across the interface in the imaginary part of the analog of the function \( \gamma \), cf. (1.13), in order to ensure the well-posedness of the problem. [13]. For a recent review of several issues regarding the interface problem for the (PE), we refer the reader to [12]; references to underwater acoustics computations with the (PE) in the presence of interfaces with change-of-variable techniques include e.g. [4, 21] and [12]. 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. [13], [20]. To alleviate this problem of energy non-conservation, change-of-variable techniques may be used as in the present paper. They may also be extended to interface, [12], or 3D-problems, [21].

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

\[
\begin{align*}
\frac{\partial u}{\partial t} & = a(t) \frac{\partial^2 u}{\partial x^2} + \beta(t, x) u + f(t, x) \quad \forall (t, x) \in [0, T] \times [0, 1], \\
u(t, 0) & = 0 \quad \forall t \in [0, T], \\
a(t) u_x(t, 1) & = \varepsilon(t) u_t(t, 1) + \delta(t) u(t, 1) + g(t) \quad \forall t \in [0, T], \\
u(0, x) & = u_0(x) \quad \forall x \in [0, 1],
\end{align*}
\]  
(1.14)

where $a(t) \geq a_* > 0$ for $t \in [0, T]$ and $\beta, f, \varepsilon, \delta, g, u_0$ are smooth, real-valued functions. Such problems occur in heat conduction, ([11], Section 4.3.5), and in other areas; see [14] 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 $\varepsilon$ in the dynamical boundary condition.

We treat first the dissipative case, characterized by the hypothesis that $\varepsilon(t) \leq 0$ for all $t \in [0, T]$, and in which the ibvp (1.14) is well posed, cf. e.g. [14]. In paragraph 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, [24], [7]. To construct a Galerkin-finite element method in this case, we replace the term $u_t$ in the dynamical boundary condition using the p.d.e. 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 paragraph 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 cf. [8].

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.,

\[ \|f\| := \left\{ \int_D |f(x)|^2 \, dx \right\}^{1/2} \quad \text{for} \quad f \in L^2(D). \]

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., $|f|_{\infty} := \text{ess sup}_D |f|$ 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.,

\[ \|f\|_s := \left\{ \sum_{\ell=0}^s \| \partial^\ell_x f \|_{2}^2 \right\}^{1/2} \quad \text{for} \quad f \in H^s(D). \]

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., $|f|_{s,\infty} := \max_{0 \leq \ell \leq s} \| \partial^\ell_x f \|_{\infty}$ 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

\[ \|v\| \leq C_{PF} |v|_{1} \quad \forall v \in \mathbb{H}^1(D), \]

the Sobolev-type inequality

\[ |v|_{\infty} \leq |v|_{1} \quad \forall v \in \mathbb{H}^1(D) \]
and the trace inequality
\[(2.3) \quad |v(1)|^2 \leq 2 \|v\|_1 |v_1| \quad \forall v \in \mathbb{H}^1(D).\]

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 non-uniform partition of \(D\) with maximum length \(h \in (0, h_\ast]\). It is well-known, \[10\], that the following approximation property holds:
\[(2.4) \quad \inf_{\chi \in S_h} \{ \|v - \chi\| + h\|v - \chi\|_1 \} \leq C h^{s+1} \|v\|_{s+1}, \quad \forall v \in \mathbb{H}^{s+1}(D), \quad \forall h \in (0, h_\ast], \quad s = 0, \ldots, r.\]

Also, we assume that the following inverse inequality holds
\[(2.5) \quad |\phi| \leq C h^{-1} \|\phi\| \quad \forall \phi \in S_h, \quad \forall h \in (0, h_\ast],\]
which is true when, for example, the partition of \(D\) is quasi-uniform, \[10\]. In addition, we define the \(L^2\)-projection operator \(P_h : L^2(D) \to S_h\) by
\[(2.6) \quad B(R_h v, \phi) = B(v, \phi) \quad \forall \phi \in S_h, \quad \forall v \in L^2(D),\]
and the elliptic projection operator \(R_h : H^1(D) \to S_h\) by
\[(2.7) \quad \|R_h v - v\| + h\|R_h v - v\|_1 \leq C h^{s+1} \|v\|_{s+1}, \quad \forall v \in \mathbb{H}^{s+1}(D), \quad \forall h \in (0, h_\ast], \quad s = 0, \ldots, r.\]

Finally, for \(v \in L^2(D)\), we define the discrete negative norm
\[(2.8) \quad \|v\|_{-1,h} := \sup \left\{ \frac{|(v, \phi)|}{\|\phi\|_1} : \phi \in S_h \quad \text{and} \quad \phi \neq 0 \right\}, \quad \forall h \in (0, h_\ast].\]

**Lemma 2.1.** The elliptic projection operator \(R_h\) has the following property:
\[(2.9) \quad R_h v(1) = v(1), \quad \forall v \in \mathbb{H}^1(D).\]

**Proof.** Let \(v \in \mathbb{H}^1(D)\) and \(\omega\) be the element of \(S_h\) given by \(\omega(x) = x\) for \(x \in \overline{D}\). Then \[(2.0)\] gives \(R_h v(1) - v(1) = B(R_h v - v, \omega) = 0\), which is the desired result. \(\square\)

**Lemma 2.2.** Let \(\omega \in C^1(\overline{D})\). Then
\[(2.10) \quad |P_h(\omega \phi)|_1 \leq C |\omega|_{1,\infty} |\phi|_1 \quad \forall \phi \in S_h, \quad \forall h \in (0, h_\ast].\]

**Proof.** Let \(h \in (0, h_\ast]\) and \(\phi \in S_h\). Since \(|P_h(\omega \phi)|_1 \leq |P_h(\omega \phi - R_h(\omega \phi))|_1 + |R_h(\omega \phi)|_1\), using \[(2.3)\] and \[(2.0)\] we arrive at \(|P_h(\omega \phi)|_1 \leq C h^{-1} |\omega \phi - R_h(\omega \phi)|_1 + |\omega \phi|_1\). Next, we use the estimate \[(2.7)\] for \(s = 0\) to obtain \(|P_h(\omega \phi)|_1 \leq C \left[ |\omega|_{\infty} |\phi|_1 + |\omega'|_{\infty} |\phi|_1 \right]\). Thus, the bound \[(2.9)\] follows by combining the latter inequality and \[(2.1)\]. \(\square\)

### 2.2. The Neumann (dynamical) boundary condition. In this subsection, we shall consider the (PE)
with the Neumann boundary condition, i.e. the ibvp \[(1.9), (1.10)\]. 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
\[(\mathcal{N}) \quad \begin{align*}
&u_t = i \alpha(t) u_{xx} + i \beta(t, x) u + f(t, x) \quad \forall (t, x) \in [0, T] \times \overline{D}, \\
&u(t, 0) = 0 \quad \forall t \in [0, T], \\
&u_x(t, 1) = \mu(t) \left[ S(t) u_x(t, 1) + G(t) u(t, 1) \right] \quad \forall t \in [0, T], \\
&u(0, x) = u_0(x) \quad \forall x \in \overline{D}.
\end{align*}\]

We shall assume that \(\alpha : [0, T] \to \mathbb{R} \setminus \{0\}\), \(\beta : [0, T] \times \overline{D} \to \mathbb{C}\), \(u_0 : \overline{D} \to \mathbb{C}\), \(\mu, S : [0, T] \to \mathbb{R}\) 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 \[(1.9), (1.10)\], and take the functions \(\alpha(t), \beta(t, x)\) as in \[(1.8)\], \(\mu(t) = \frac{\mu_0(t)}{\mu(t)}\), \(S(t) = \frac{S(t)}{S(t)}\), \(G(t) = g(t) S(t) + i \left[ S(t) \delta(t) - s^2(t) \right]\), where \(\delta = \frac{\alpha(t)}{\beta(t, x)}\).)
2.2.1. Semidiscrete approximation. The weak formulation of \((\mathcal{N})\), obtained by taking the \(L^2(D)\) inner product of the p.d.e. in \((\mathcal{N})\) with a function in \(H^1(D)\), 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

\[
(\partial_t u_h(t, \cdot), \phi) = i a(t) \mu(t) \left[ S(t) \partial_t \theta_h(t, 1) + G(t) u_h(t, 1) \right] \phi(1) - i a(t) B(u_h(t, \cdot), \phi) + i (\beta(t, \cdot) u_h(t, \cdot), \phi) + (f(t, \cdot), \phi) \quad \forall \phi \in S_h, \quad \forall t \in [0, T],
\]

where \(\varphi \in C^1([0, T]; S_h)\) is subject to the boundary conditions (2.13).

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. Then, we have \(R_h u_0 = \sum_{j=1}^J \gamma_j^0 \phi_j\) and \(u_h(t, x) = \sum_{j=1}^J \gamma_j(t) \phi_j(x)\), where \(\gamma_j : [0, T] \to \mathbb{C}\) for \(j = 1, \ldots, J\). Then (2.10) - (2.11) is equivalent to the following o.d.e. initial-value problem: Find \(\tilde{G} \in C^1([0, T]; \mathbb{C})\) such that \(\tilde{G}(0) = \tilde{G}^0\) and \(\tilde{A}(t) \tilde{G}(t) = \tilde{B}(t) \tilde{F}(t), \quad \forall t \in [0, T]\), where \(\tilde{G}(t) := (\gamma_1(t), \ldots, \gamma_J(t))^T\), \(\tilde{G}^0 := (\gamma_1^0, \ldots, \gamma_J^0)^T\), \(\tilde{A} : [0, T] \to \mathbb{C}^{J \times J}\) with \(\tilde{A}_J(t) := (\phi_j(t, \cdot), \phi_j(t) - i a(t) S(t) \mu(t) \phi_j(t), 1, \tilde{B} : [0, T] \to \mathbb{C}^{J \times J}\) with \(\tilde{B}_J(t) := i a(t) G(t) \mu(t) \phi_j(t), 1, 1 - i a(t) B(\phi_j(t, \cdot), \phi_j(t) - i a(t) S(t) \mu(t) \phi_j(t), 1, \tilde{F} : [0, T] \to \mathbb{C}\) with \(\tilde{F}(t) := (f(t, \cdot, \phi_1), \ldots, (f(t, \cdot, \phi_J))^T\). Since \(\tilde{A}, \tilde{B}, \tilde{F}\) are continuous maps, to ensure existence and uniqueness of the solution \(\tilde{G}\), it is sufficient to show that \(\tilde{A}(t)\) is nonsingular for \(t \in [0, T]\). Indeed, letting \(t \in [0, T]\) and \(x \in \text{Ker}(\tilde{A}(t))\), we have \(\text{Re}(\tilde{F}(t)) = 0\), from which we conclude that \(\|\sum_{j=1}^J x_j \phi_j\|^2 = 0\) and hence \(x = 0\). □

Let us first present a \(H^1\) superconvergence error estimate for the semidiscrete approximation \(u_h\).

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

\[
\|u_h(t, \cdot) - R_h u(t, \cdot)\|_1 \leq C h^{r+1} \left( \int_0^t \Gamma_x(\tau) \, d\tau \right)^{\frac{1}{2}} \quad \forall t \in [0, T], \quad \forall h \in (0, h_*)
\]

where \(\Gamma_x(\tau) := \|u(\tau, \cdot)\|_{L^2}^2 + \|\partial_t u(\tau, \cdot)\|_{L^2}^2 + \sum_{s=0}^r \int_0^\tau \|\partial_s^r u(s, \cdot)\|_{L^2}^2 \, ds\).

Proof. Let \(h \in (0, h_*)\), \(\theta_h := u_h - R_h u\) and \(\xi(t) := \frac{1}{a(t)}\). Using (2.6) and (2.5) we obtain

\[
(\partial_t \theta_h(t, \cdot), \phi) = i a(t) \mu(t) \left[ S(t) \partial_t \theta_h(t, 1) + G(t) \theta_h(t, 1) \right] \phi(1) - i a(t) B(\theta_h(t, \cdot), \phi) + i (\Psi_*(t, \cdot), \phi) \quad \forall \phi \in S_h, \quad \forall t \in [0, T],
\]

where \(\Psi_* := [\partial_t \theta_h - R_h \partial_t \theta_h] - i \beta(u - R_h u)\). Set \(\phi = \partial_t \theta_h\) in (2.13) and then take imaginary parts to obtain

\[
\begin{align*}
\frac{d}{dt} \|\theta_h(t, \cdot)\|^2 & \leq |\mu(t)| \left[ - 2 S^* \|\partial_t \theta_h(t, 1)\|^2 + 2 |G(t)| \|\theta_h(t, 1)\| \|\partial_t \theta_h(t, 1)\| \right] \\
& + 2 \|\xi(t)\| \|\partial_t \theta_h(t, \cdot)\|^2_{-1, h} \|P_h(\beta(t, \cdot) \theta_h(t, \cdot), \cdot)\|_{1, h} \\
& + 2 \|\xi(t)\| \|P_h(\beta(t, \cdot) \theta_h(t, \cdot), \cdot)\|_{1, h} \|\theta_h(t, \cdot)\|_{-1, h} \quad \forall t \in [0, T],
\end{align*}
\]

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

\[
\|\Psi_*(t, \cdot)\| \leq C h^{r+1} \left[ \|u(t, \cdot)\|_{L^2} + \|\partial_t u(t, \cdot)\|_{L^2} \right] \quad \forall t \in [0, T].
\]

Then, use of (2.2) and (2.15) in (2.13) gives

\[
\|\partial_t \theta_h(t, \cdot)\|^2 \leq \|a(t)\| \left[ S(t) \|\mu(t)\| \|\partial_t \theta_h(t, 1)\| + \left( |G(t)| |\mu(t)| + 1 \right) \|\theta_h(t, \cdot)\|_{1, h} \right] \|\phi\|_1 \\
+ |\beta(t, \cdot)| \|\theta_h(t, \cdot)\| \|\phi\|_1 \\
+ C h^{r+1} \left[ \|\partial_t u(t, \cdot)\|_{L^2} + \|u(t, \cdot)\|_{L^2} \right] \|\phi\| \quad \forall \phi \in S_h, \quad \forall t \in [0, T],
\]
which, along with (2.1), yields that
\[ 2|ξ(t)| \|
abla \theta_h(t, ·)\|_{-1, h} \leq 2S(t) \|μ(t)\| \|D \theta_h(t, 1)\| \]
\[ + C \left[ \|\theta_h(t, ·)\|_{1} + h^{r+1} \left( \|\partial_t u(t, ·)\|_{r+1} + \|u(t, ·)\|_{r+1} \right) \right] \quad \forall t \in [0, T]. \]

(2.16)

Thus, combining (2.14), (2.19), (2.1), and (2.2), we arrive at
\[ \frac{d}{dt} |\theta_h|^2 \leq C \left[ |\theta_h|^2 + h^{2(r+1)} \left( \|\partial_t u\|_{r+1}^2 + \|u\|_{r+1}^2 \right) \right] + 2 \xi \text{Im}(Ψ_*, D \theta_h) \quad \text{on } [0, T]. \]

Since \( \theta_h(0, ·) = 0 \), integrating with respect to \( t \) in the inequality above yields
\[ |\theta_h(t, ·)|^2 \leq C \int_0^t |\theta_h(s, ·)|^2 ds + C h^{2(r+1)} \Gamma_{X'}(t) \quad \forall t \in [0, T]. \]

(2.17)

The estimate (2.12) follows from (2.17) using Grönwall’s lemma and (2.1).

□

A simple consequence of this superconvergence estimate and the approximation property (2.7) of the elliptic projection is the following convergence result:

**Theorem 2.5.** Let \( u \) be the solution of (N) and \( u_h \) its semidiscrete approximation defined by (2.10)-(2.11). Assume that \( μ(t) \leq 0 \) and \( S(t) > 0 \) for \( t \in [0, T] \). Then

\[ \|u_h(t, ·) - u(t, ·)\| + h \|u_h(t, ·) - u(t, ·)\|_1 \leq C h^{r+1} \left( \|u(t, ·)\|_{r+1} + \int_0^t \Gamma_{X'}(τ) \, dτ \right) \quad \forall t \in [0, T], \]

(2.18)

where \( \Gamma_{X'} \) is the function defined in the statement of Proposition 2.4.

□

Therefore, 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 2.5 holds in the case of domains with upsloping bottom profiles, i.e., when \( s(t) \leq 0 \) for \( t \in [0, T] \).

**Remark 2.1.** The \( H^1 \) superconvergence estimate (2.12), (2.2), and a standard \( L^\infty \) estimate for the error of the elliptic projection (2.5) yield as usual an optimal-order estimate of the error \( |u - u_h|_\infty \) on \( [0, T] \) (cf. 2.9).

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 \( n = 0, \ldots, N - 1 \). Define \( k_n := t^n - t^{n-1} \) for \( n = 1, \ldots, N \) and \( \frac{t^n}{2} := \frac{t^n - t^{n+1}}{2} \) for \( n = 1, \ldots, N - 1 \), and \( k := \max_{1 \leq n \leq N} k_n \). We set \( u^n := u(t^n, ·) \) for \( n = 0, \ldots, N \), where \( u \) is the solution of (N). Finally, for sequences \( (V^m)_{m=0}^M \), we define \( \partial V^m := \frac{1}{k_n} (V^m - V^{m-1}) \) and \( AV^m = \frac{1}{2} (V^m + V^{m-1}) \) for \( m = 1, \ldots, M \).

For \( n = 0, \ldots, N \), the Crank-Nicolson method yields an approximation \( U^n_h \in S_h \) of \( u(t^n, ·) \) as follows:

**Step 1:** Set
\[ U^0_h := R_h u_0. \]

(2.19)

**Step 2:** For \( n = 1, \ldots, N \), find \( U^n_h \in S_h \) such that
\[ (\partial U^n_h, χ) = i a_n - \frac{1}{2} μ_n - \frac{1}{2} \left[ S_n^{-\frac{1}{2}} \partial U^n_h(1) + G_n^{-\frac{1}{2}} AU^n_h(1) \right] χ(1) \]
\[ - i a_n - \frac{1}{2} B (AU^n_h, χ) + i (β_n - \frac{1}{2} AU^n_h, χ) + (f_n - \frac{1}{2}, χ) \quad \forall χ \in S_h, \]

(2.20)

where \( S_n^{-\frac{1}{2}} := S(t^n - \frac{1}{2}), μ_n - \frac{1}{2} := μ(t^n - \frac{1}{2}), a_n - \frac{1}{2} := a(t^n - \frac{1}{2}), G_n^{-\frac{1}{2}} := G(t^n - \frac{1}{2}), f_n - \frac{1}{2} := f(t^n - \frac{1}{2}, ·) \) and \( β_n - \frac{1}{2} := β(t^n - \frac{1}{2}, ·) \).
We first examine the problem of existence and uniqueness of the fully discrete approximation $U^n_h$.

**Proposition 2.6.** Let $n \in \{1, \ldots, N\}$ and suppose that $U^{n-1}_h \in S_h$ is well defined. If $S^{n-\frac{1}{2}} > 0$ and $\mu^{n-\frac{1}{2}} \leq 0$, then, there exists a constant $C_n$ such that if $k_n < C_n$, then $U^n_h$ is well defined by (2.20).

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

\[
\frac{1}{k_n}(V, \phi) = i a^{n-\frac{1}{2}} \mu^{n-\frac{1}{2}} \left[ S^{n-\frac{1}{2}} \frac{1}{k_n} V(1) + G^{n-\frac{1}{2}} \frac{1}{2} V(1) \right] \phi(1)
- i \frac{a^{n-\frac{1}{2}}}{2} B(V, \phi) + \frac{1}{2} (P_h(\beta^{n-\frac{1}{2}}, V), \phi) \quad \forall \phi \in S_h,
\]

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

\[
|V|_1^2 = \mu^{n-\frac{1}{2}} k_n \left[ \frac{2 S^{n-\frac{1}{2}}}{k_n} \left| \frac{V(1)}{k_n} \right|^2 + \frac{k_n}{a^{n-\frac{3}{2}}} \text{Re}(G^{n-\frac{1}{2}}) |V(1)|^2 \right] \leq |\mu^{n-\frac{1}{2}}| k_n \left[ \frac{2 S^{n-\frac{1}{2}}}{k_n} \left| \frac{V(1)}{k_n} \right|^2 + \frac{k_n}{a^{n-\frac{3}{2}}} \text{Re}(P_h(\beta^{n-\frac{1}{2}}, V), V) \right].
\]

For $\phi \in S_h$, we use (2.21), (2.22) and (2.9) to obtain

\[
| \frac{V}{k_n} |_{-1, h} \leq |\alpha|^{n-\frac{3}{2}} |\mu^{n-\frac{1}{2}}| \left[ S^{n-\frac{1}{2}} \left| \frac{V(1)}{k_n} \right| + |G^{n-\frac{1}{2}}| \frac{1}{2} |V(1)| \right] |\phi|_1
+ \frac{1}{2} \left[ |\alpha n^{-\frac{1}{2}} + C |\beta^{n-\frac{1}{2}}| \right] |V|_1 |\phi|_1,
\]

which yields

\[
\frac{|V|}{k_n} \leq |\alpha|^{n-\frac{3}{2}} |\mu^{n-\frac{1}{2}}| S^{n-\frac{1}{2}} \left| \frac{V(1)}{k_n} \right| + C_e |V|_1,
\]

where $C_e := \frac{1}{2} \left[ |\alpha|^{n-\frac{3}{2}} + C |\beta^{n-\frac{1}{2}}| + |\alpha|^{n-\frac{1}{2}} |\mu^{n-\frac{1}{2}}| |G^{n-\frac{1}{2}}| \right]$. Using (2.22) and (2.23), (2.7) gives

\[
|V|^2 \left\{ 1 - k_n \left[ \frac{1}{2} \left[ |\alpha|^{n-\frac{3}{2}} + C e |\beta^{n-\frac{1}{2}}| + C e |\mu^{n-\frac{1}{2}}| S^{n-\frac{1}{2}} \left| \frac{V(1)}{k_n} \right| \right] \right] \right\} \leq 0,
\]

which ends the proof. □

In particular, if we suppose that $\beta$ is in $C([0, T], W^{1, \infty}(D))$, that $a$, $\mu$, $S$, $G$ are continuous functions on $[0, T]$, and that $S(t) > 0$ and $\mu(t) \leq 0$ for $t \in [0, T]$ (i.e. the upsloping case), then the existence and uniqueness of the fully discrete approximation $U^n_h$ follows if $k_n \leq C$, where $C$ is a constant independent of $n$. This follows from Proposition 2.6 and the fact that the quantity multiplying $k_n$ in (2.24) may be uniformly bounded with respect to $n$.

In the case of a general bottom topography we have:

**Proposition 2.7.** Let $n \in \{1, \ldots, N\}$ and suppose that $U^{n-1}_h \in S_h$ is well defined. Then, there exist constants $C_{n, 1}$ and $C_{n, 2}$ such that if $k_n < C_{n, 1}$ and $k_n < C_{n, 2}$, then $U^n_h$ is well defined by (2.20).

**Proof.** 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 $U^n_h$ is equivalent to the invertibility of a matrix $\widetilde{M} \in \mathbb{C}^{J \times J}$ defined by $\widetilde{M}_{ij} := \mathcal{M}(\phi_j, \phi_i)$ for $j, \ell = 1, \ldots, J$, where $\mathcal{M} : S_h \times S_h \to \mathbb{C}$ is given by $\mathcal{M}(\chi, \phi) := (\chi, \phi) - i a^{n-\frac{1}{2}} \mu^{n-\frac{1}{2}} S^{n-\frac{1}{2}} \chi(1) \phi(1) + \frac{k_n}{2} \left[ -i (\beta^{n-\frac{1}{2}}, \chi, \phi) - i \mu^{n-\frac{1}{2}} a^{n-\frac{1}{2}} G^{n-\frac{1}{2}} \chi(1) \phi(1) \right]$ for $\chi, \phi \in S_h$. If $x \in \text{Ker}(\widetilde{M})$ we have $\text{Re} [\mathcal{M}(\phi, \phi_*)] = 0$ with $\phi_* := \sum_{j=1}^J x_j \phi_j$. Then, using (2.20) and (2.28), we get

\[
\|\phi_*\|^2 \leq \frac{k_n}{2} \left[ |\beta^{n-\frac{1}{2}}| \|\phi_*\|^2 + 2|\mu^{n-\frac{1}{2}}| |a^{n-\frac{1}{2}}| |G^{n-\frac{1}{2}}| \|\phi_*\| \|\phi_*\| \right],
\]

which, under our hypotheses, yields $x = 0$ and ends the proof. □
Hence, if $\beta \in C([0,T], L^{\infty}(D))$ and $a, \mu, G$ are continuous on $[0,T]$ (i.e. in the case of general bottom topography), the existence and uniqueness of $U_h$ follows if we take $k_n \leq C_1$ and $\frac{h}{k_n} \leq C_2$, for some constants $C_1$ and $C_2$ independent of $n$.

We next establish the consistency of our fully discrete scheme in the $t$ variable.

**Proposition 2.8.** Let $u$ be the solution of (N). For $n = 1, \ldots, N$, define $\sigma^n : \mathbb{T} \rightarrow \mathbb{C}$ by

$$\frac{u^n - u^{n-1}}{k_n} = i a^{n-\frac{1}{2}} u_{xx}(t^{n-\frac{3}{2}}, \cdot) + i \beta^{n-\frac{1}{2}}Au^n + f^{n-\frac{1}{2}} + \sigma^n.$$  

Then,

$$\|\sigma^n\| \leq C (k_n)^2 B_1^n(u), \quad n = 1, \ldots, N,$$

$$\|\sigma^{n+1} - \sigma^n\| \leq C \left[ (k_n)^2 + |k_n| \right] (k_n + k_{n+1}) B_2^n(u), \quad n = 1, \ldots, N - 1,$$

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

**Proof.** It follows easily by using the partial differential equation and Taylor’s formula. □

We prove now that the following $H^1$ superconvergence estimate holds in the fully discrete case.

**Proposition 2.9.** Let $u$ be the solution of (N) and $(U^n_h)_{n=0}^N$ be the fully discrete approximations that the method (2.19) - (2.20) produces. Assume that $\mu(t) \leq 0$ and $S(t) > 0$ for $t \in [0,T]$. In addition, assume that there exists a constant $C \geq 0$ such that

$$|k_{n+1} - k_n| \leq C \max_{1 \leq n \leq N} \left\{ k_n^2, k_{n+1}^2 \right\}, \quad n = 1, \ldots, N - 1.$$

Then, there exists a constant $C_1$ such that, if $\max_{1 \leq n \leq N} (k_n C_1) \leq \frac{1}{4}$, there exists a constant $C > 0$ such that

$$\max_{1 \leq n \leq N} \|U^n_h - R_h u^n\| \leq C (k_n^2 + h^{r+1}) \Xi_n(u) \quad \forall h \in (0, h_*],$$

where $\Xi_n(u) := \sum_{t=2}^{2} \max_{[t, t]} \|\partial_t u\| + \max_{[t, t]} \|\partial_t^2 u\| + \max_{[t, t]} \|\partial_t^4 u(t, 1)\|$.

**Proof.** Let $h \in (0, h_*]$, $\theta^n_h := U^n_h - R_h u^n$ for $n = 0, \ldots, N$, $\xi := \frac{1}{2}$ and $\xi^{n-\frac{1}{2}} := \xi(t^{n-\frac{1}{2}})$ for $n = 1, \ldots, N$. We use (2.20), (2.25), (2.6), and (2.8), to obtain

$$\begin{align*}
(\partial \theta_h^n, \chi) &= i a^{n-\frac{1}{2}} \mu^{n-\frac{1}{2}} \left[ S^{n-\frac{1}{2}} \partial \theta_h^n(1) + G^{n-\frac{1}{2}} \partial \theta_h^n(1) - \xi^n \right] \chi(1) \\
&= i a^{n-\frac{1}{2}} B(\theta_h^n, \chi) + i (P_h(\beta^{n-\frac{1}{2}} A \theta_h^n), \chi) \\
&+ (\xi^n - \sigma^n, \chi) + i a^{n-\frac{1}{2}} B(\xi^n, \chi) \quad \forall \chi \in Q_h, \quad n = 1, \ldots, N,
\end{align*}$$

where

$$\begin{align*}
\xi^n &:= \partial u^n - R_h(\partial u^n) - i P_h[\beta^{n-\frac{1}{2}} (Au^n - R_h(Au^n))], \\
\xi_2^n &:= u(t^{n-\frac{1}{2}}) - Au^n, \\
\xi_3^n &:= S^{n-\frac{1}{2}} [\partial_t u(t^{n-\frac{1}{2}}, 1) - u^n(1)] + G^{n-\frac{1}{2}} [u(t^{n-\frac{1}{2}}, 1) - Au^n(1)].
\end{align*}$$

Using Taylor’s formula and (2.27), we deduce the following estimates:

$$\|\xi_1^n\| \leq C \frac{h^{r+1}}{k_n} \left( \int_{t^{n-1}}^{t^n} \|\partial_t u(s, \cdot)\| ds \right)_{t^{r+1}} + C |\beta^{n-\frac{1}{2}}|_\infty h^{r+1} \|Au^n\|_{t^{r+1}}$$

$$\leq C h^{r+1} \left( \max_{[t^{n-1}, t^n]} \|u\|_{t^{r+1}} + \max_{[t^{n-1}, t^n]} \|\partial_t u\|_{t^{r+1}} \right),$$

$$|\xi_2^n| \leq C k_n^2 \max_{[t^{n-1}, t^n]} \|\partial_t^2 u(t, 1)\|,$$

and

$$|\xi_3^n| \leq C k_n^2 \max_{[t^{n-1}, t^n]} \|\partial_t^3 u(t, 1)\| + \max_{[t^{n-1}, t^n]} \|\partial_t^2 u(t, 1)\|.$$
where $\Xi^C$ from which there follows that for some constant $\lambda$

$$
(2.34) \quad + k_n |\mu^{n-\frac{1}{2}}| \left[ -2 S_n |\partial \theta^0_n(1)|^2 + 2 |G^{n-\frac{1}{2}}| |A \theta^0_n(1)| |\partial \theta^0_n(1)| + 2 |E^0_n| |\partial \theta^0_n(1)| \right] + 2 k_n \Re[\mathcal{B}(E^0_n, \partial \theta^0_n)] + 2 k_n \xi^{n-\frac{1}{2}} \Im(E^0_n - \sigma^n, \partial \theta^0_n), \quad n = 1, \ldots, N,
$$

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

Now let us estimate $\|\partial \theta^0_n\|_{-1,h}$. For $\varphi \in S_h$, $\|\partial \theta^0_n\|_{-1,h}$, $\|\partial \theta^0_n\|_{1}$, and $\|\partial \theta^0_n\|_{1}$ give

$$
\|\partial \theta^0_n \| \leq |\xi^{n-\frac{1}{2}}| |\partial \theta^0_n| \|\partial \theta^0_n(1)| |\varphi|_1 + C |A \theta^0_n| |\varphi|_1 + C (h^{r+1} + k_n^2) |\varphi|_1 \Xi_1(u), \quad n = 1, \ldots, N,
$$

where $\Xi_1(u) := \max_{[0,T]} \|u\|_{r+1} + \max_{[0,T]} \|\partial u\|_{r+1} + \max_{[0,T]} \|\partial^2 u\|_1 + \max_{[0,T]} \|\partial^3 u\| + \max_{t\in[0,T]} |\partial^4 u(t, 1)|$.

Hence, we conclude that

$$
(2.35) \quad 2 k_n |\xi^{n-\frac{1}{2}}| |\partial \theta^0_n| \|\partial \theta^0_n(1)| + C k_n |A \theta^0_n| + C k_n (h^{r+1} + k_n^2) \Xi_1(u), \quad n = 1, \ldots, N.
$$

Now, combining (2.35) and (2.34) we have

$$
(2.36) \quad (1 - C_1 k_n) |\theta^0_n|_1^2 \leq (1 + C_1 k_n) |\theta^0_n|_1^2 + C_2 k_n (h^{r+1} + k_n^2)^2 (\Xi_1(u))^2 + 2 k_n \Re[\mathcal{B}(E^0_n, \partial \theta^0_n)] + 2 k_n \xi^{n-\frac{1}{2}} \Im(E^0_n - \sigma^n, \partial \theta^0_n), \quad n = 1, \ldots, N.
$$

To continue, we assume that $\max_{1 \leq n \leq N} (C_1 k_n) \leq \frac{1}{3}$, which allows us to conclude that $\frac{1+C_1 k_n}{1-C_1 k_n} \leq e^{3C_1 k_n}$ for $n = 1, \ldots, N$. Hence, (2.36) yields

$$
|\theta^0_n|_1^2 \leq e^{3C_1 k_n} |\theta^0_n|_1^2 + \frac{C_2 k_n}{1-C_1 k_n} (h^{r+1} + k_n^2)^2 (\Xi_1(u))^2 + 2 k_n \Re[\mathcal{B}(E^0_n, \partial \theta^0_n)] + 2 k_n \xi^{n-\frac{1}{2}} \Im(E^0_n - \sigma^n, \partial \theta^0_n), \quad n = 1, \ldots, N.
$$

Next, we define $\lambda^j_n := \frac{\exp(3C_1 \sum_{1 \leq j \leq n} k_j)}{1-C_1 k_j}$ and use a simple induction argument to arrive at

$$
|\theta^0_n|_1^2 \leq C_2 (\Xi_1(u))^2 \sum_{j=1}^n k_j \lambda^j_n (h^{r+1} + k^2_j)^2 + 2 \sum_{j=1}^n k_j \lambda^j_n \left[ \Re[\mathcal{B}(E^0_j, \partial \theta^0_j)] + \xi^{j-\frac{1}{2}} \Im(E^0_j - \sigma^j, \partial \theta^0_j) \right], \quad n = 1, \ldots, N,
$$

which yields

$$
(2.37) \quad |\theta^0_n|_1^2 \leq C (h^{r+1} + k^2)^2 (\Xi_1(u))^2 + T^a_n + T^b_n, \quad n = 1, \ldots, N,
$$

where

$$
T^a_n := 2 \sum_{j=1}^n \lambda^j_n \Re[\mathcal{B}(E^0_j, \partial \theta^0_j - \theta^0_j)],
$$

$$
T^b_n := 2 \sum_{j=1}^n \lambda^j_n \xi^{j-\frac{1}{2}} \Im(E^0_j - \sigma^j, \theta^0_j - \theta^0_j^{-1}).
$$
Proof. It is a simple consequence of (2.29) and (2.7). □
We conclude that in the case of upsloping bottoms, the fully discrete Crank-Nicolson-Galerkin method (2.19), (2.20) yields fully discrete approximations $U_h^n$ that converge to the solution $u$ of $(N)$ at optimal rates in the $L^2$ and $H^1$ norms.

2.3. The Abrahamsson-Kreiss boundary condition. We consider now the (PE) with the Abrahamsson-Kreiss bottom boundary condition, i.e. the ibvp (1.9), (1.8), (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

\begin{align*}
  u_t &= i a(t) u_{xx} + 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{align*}

(ÅK)

We assume again that $a : [0, T] \to \mathbb{R} \setminus \{0\}$, $\beta, f : [0, T] \times \overline{D} \to \mathbb{C}$, $u_0 : \overline{D} \to \mathbb{C}$ are given functions. We shall assume that the solution of (ÅK) exists uniquely and that the data and the solution of (ÅK) are smooth enough for the purposes of the error estimation. We note that (ÅK) may be considered as a special case of (N) obtained by setting $\mu$ equal to zero in (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 $\beta$, cf. (1.7), and in the change-of-variable formula (1.5).) All the error estimates for (ÅK) that follow may then be considered as special cases of the analogous estimates in the two preceding paragraphs but with some important simplifications. For the convenience of the reader we shall restate the results but not prove them in detail; we shall just point out some differences between them and the analogous estimates for the problem (N). It will be seen that the finite element approximations of (ÅK) exist and 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 paragraph 2.1 we define the semidiscrete approximation $u_h$ of the solution of (ÅK) as the map $u_h : [0, T] \to S_h$ satisfying

\begin{align*}
  (\partial_t u_h(t, \cdot), \phi) &= -i a(t) B(u_h(t, \cdot), \phi) + 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], \\
  u_h(0, \cdot) &= u_0^h,
\end{align*}

(2.43)

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

**Proposition 2.11.** The problem (2.43), (2.44) admits a unique solution in $C^1([0, T], S_h)$. If $f \equiv 0$ and $\beta_1 \equiv 0$, then the solution preserves the $L^2(D)$ norm, i.e.,

\begin{equation}
  \|u_h(t, \cdot)\| = \|u_0^h\| \quad \forall t \in [0, T].
\end{equation}

(2.45)

**Proof.** The first part follows from Proposition 2.3 for $\mu = 0$. The conservation of the $L^2(D)$ norm follows by taking $\phi = u_h$ in (2.43) and then real parts. $\square$

**Theorem 2.12.** Let $u$ be the solution of (ÅK) and $u_h$ its semidiscrete approximation defined by (2.43)-(2.44). Then

\begin{equation}
  \|u(t, \cdot) - u_h(t, \cdot)\|_\ell \leq C \left( \|u_0^h\| - R_h u_0\|_\ell + h^{r+1-\ell} \left( \|u(t, \cdot)\|_{r+1}^2 + \int_0^t \Gamma_{\text{ÅK}, \epsilon}(\tau) d\tau \right) \right)^{1/2} \quad \forall t \in [0, T],
\end{equation}

(2.46)

for $\ell = 0, 1$ and $h \in (0, h_\star]$, where $\Gamma_{\text{ÅK}, \epsilon}(\tau) := \sum_{r=0}^\infty \|\partial_\tau^r u(\tau, \cdot)\|_{r+1}^2$ and $\Gamma_{\text{ÅK}, \epsilon}(\tau) := \Gamma_{\epsilon}(\tau)$, where $\Gamma_{\epsilon}$ is the function defined in the statement of Proposition 2.4.
Proof. Let $h \in (0, h_*]$. Defining as usual $\theta_h := u_h - R_h u$ we obtain
\begin{equation}
(2.47) \quad (\partial_t \theta_h(t, \cdot), \phi) = -ia(t) B(\theta_h(t, \cdot), \phi) + i(\beta(t, \cdot) \theta_h(t, \cdot), \phi) + (\Psi_s(t, \cdot), \phi) \quad \forall \phi \in S_h, \quad \forall t \in [0, T],
\end{equation}
where $\Psi_s$ was defined in the course of the proof of Proposition 2.14. Taking $\phi = \theta_h$ in (2.47) and then real parts, we may prove (2.46) with $\ell = 0$ in a straightforward manner. The proof of (2.46) with $\ell = 1$ follows the steps of the proof of Proposition 2.14 if we take $\phi = \partial_t \theta_h$ in (2.47) and then imaginary parts. □

Remark 2.2. Hence, if $u^0_h$ is taken equal to $P_h u^0$ or $R_h u^0$, Theorem 2.13 yields optimal-order estimates of the error $u - u_h$ in the $L^2$ or $H^1$ norm, respectively. Also, we note that to obtain the estimate (2.46) with $\ell = 0$, we do not need the inverse inequality (2.5).

2.3.2. Crank-Nicolson fully discrete approximations. We now proceed to the full discretization of $(\mathcal{A}K)$ by discretizing the initial-value problem (2.43)-(2.44) in $t$ using the Crank-Nicolson scheme. With notation introduced in paragraph 2.2.2, we define for $n = 0, \ldots, N$ approximations $U^n_h \in S_h$ of $u(t^n, \cdot)$, the solution of $(\mathcal{A}K)$, as follows:

Step 1: Set
\begin{equation}
(2.48) \quad U^0_h := u^0_h.
\end{equation}

Step 2: For $n = 1, \ldots, N$, find $U^n_h \in S_h$ such that
\begin{equation}
(2.49) \quad (\partial U^n_h, \chi) = -i a^n \frac{1}{2} B(\mathcal{A}U^n_h, \chi) + i (\beta^n \frac{1}{2} A \mathcal{U}U^n_h, \chi) + (f^n, \chi) \quad \forall \chi \in S_h.
\end{equation}

Proposition 2.13. Let $n \in \{1, \ldots, N\}$ and suppose $U^n_h^{-1}$ is well defined. Then, there exists a constant $C$ independent of $n$ such that if $k_n \leq C$, $U^n_h$ is well defined by (2.49). Moreover, if $f \equiv 0$ and $\beta_t \equiv 0$, then
\begin{equation}
(2.50) \quad ||U^n_h|| = ||u^0_h||, \quad n = 0, \ldots, N.
\end{equation}

Proof. Since (2.49) is equivalent to a $\dim(S_h) \times \dim(S_h)$ linear system of algebraic equations, existence and uniqueness of $U^n_h$ will follow if we show that if there is a $V \in S_h$ such that
\begin{equation}
(2.51) \quad \frac{1}{k_n}(V, \phi) = -\frac{i}{2} a^n \frac{1}{2} B(V, \phi) + i (\beta^n \frac{1}{2} V, \phi) \quad \forall \phi \in S_h,
\end{equation}
then $V = 0$. This fact follows easily for $k_n$ sufficiently small, if we put $\phi = V$ in (2.51) and take real parts. The conservation property (2.50) follows from (2.49) if we select $\chi = \mathcal{A}U^n_h$ and take real parts. □

Theorem 2.14. Let $u$ be the solution of $(\mathcal{A}K)$ and $(U^n_h)_{n=0}^{N}$ be the fully discrete approximations produced by (2.48)-(2.49). Then, if $\max_{1 \leq n \leq N} k_n$ is sufficiently small, we have
\begin{equation}
(2.52) \quad \max_{0 \leq n \leq N} \|U^n_h - u^n\| \leq C \left[ \|u^0_h - R_h u_0\| + (k^2 + h^{r+1}) \Xi_{\mathcal{A}K, 0}(u) \right] \quad \forall h \in (0, h_*],
\end{equation}
where $\Xi_{\mathcal{A}K, 0}(u) := \sum_{m=0}^{3} \max_{[0, T]} \|\partial_t^m u\|_{r+1} + \sum_{m=2}^{3} \max_{[0, T]} \|\partial_t^m u\| + \max_{[0, T]} \|\partial_t^2 u\| = \max_{[0, T]} \|\partial_t^2 u\|$. Also, if (2.50) and (2.28) hold, and $\max_{1 \leq n \leq N}$ $k_n$ is sufficiently small, then
\begin{equation}
(2.53) \quad \max_{0 \leq n \leq N} \|U^n_h - u^n\| \leq C \left[ \|u^0_h - R_h u_0\| + 1 \right] \Xi_{\mathcal{A}K, 1}(u) \quad \forall h \in (0, h_*],
\end{equation}
where $\Xi_{\mathcal{A}K, 1}(u) := \Xi_{\mathcal{A}K, 0}(u) + \max_{[0, T]} \|\partial_t^2 u\|_{r+1} + \max_{[0, T]} \|\partial_t^4 u\| + \max_{[0, T]} \|\partial_t^4 u\|$. □

Proof. First, we modify the consistency argument of Proposition 2.8 defining, for $n = 1, \ldots, N$, $\sigma^n : \overline{D} \to \mathbb{C}$ by $\sigma^n := a^n \frac{1}{2} A(\mathcal{A}u(t^n, \cdot)) + 1 \beta^n \frac{1}{2} A\mathcal{U}u + f^n \frac{1}{2} + \sigma^n$. Then, we set $\theta^n_h := U^n_h - R_h u^n$ for $n = 0, \ldots, N$, to obtain (2.30) simplified by setting $\mu^n = 0$ and $E^n_0 = 0$. To obtain (2.52) we put $\chi = \theta^n_h$ and then take real parts. To obtain (2.53) we proceed along the lines of the proof of Proposition 2.9 appropriately simplified. □
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 paragraph 3.3, a theoretical excursion with the aim of explaining some experimental observations made in paragraph 3.2. Recall that in the case of the Neumann boundary condition, i.e. for the problem \( (N) \), our convergence results were rigorously established in the case of upsloping bottoms, that is when \( s(t) \leq 0 \) 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 \( (N) \) 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. Order of convergence. To test numerically the order of convergence of the fully discrete Crank-Nicolson-Galerkin finite element method (henceforth referred to as (FE)) in the case of the ibvp \( (N) \), we took \( T = 1 \) and considered three cases of bottom profiles, namely:

- Case 1: \( s(t) = -0.3t + 0.7 \) (upsloping).
- Case 2: \( s(t) = 0.4t + 0.3 \) (downsloping).
- Case 3: \( s(t) = 0.2 \cos(4\pi t) + 0.2 \sin(4\pi t) + 0.7 \) (oscillatory).

In \( (N) \) we took \( \alpha = 1/(2s^2) \), \( \beta(t, x) = xt + i(3x + t^2) \), \( u_0(x) = -x(x - 1)^3 \). The bottom boundary condition had the form \( u_x(t, 1) = \mu(t) [S(t)u(t, 1) + G(t)u(t, 1)] + f_1(t) \), where \( \mu(t) = \frac{s(t)}{s(t)} \), \( S(t) = \frac{s^2(t)}{1 + (s(t))^2} \), \( G(t) = i(S(t)\dot{s}(t) - s^2(t)) \), \( \delta = ss/2 \). The nonhomogeneous terms \( f \) and \( f_1 \) were chosen so that the exact solution of the problem was given by \( u(t, x) = -x(x - 1)^3 + \sin(t) x \). To compare the exact with the numerical solution we calculated the \( l_2 \) error at the nodes \( x_j \) at \( T = 1 \) (taking \( k = h \)). Table 4.1 shows the rates of convergence of the numerical solution in the three cases. The rate is clearly two in the upsloping case.

| \( h \) | Case 1 | Case 2 | Case 3 |
|---|---|---|---|
| 1/100 | 1.998 | 1.638 | 1.766 |
| 1/200 | 1.999 | 1.659 | 1.085 |
| 1/400 | 1.999 | 2.001 | 1.556 |
| 1/800 | 2.000 | 2.012 | 2.615 |

Table 4.1. Orders of convergence of (FE) for \( (N) \) in \( l_2 \) in three cases of bottom topography.

3.2. Comparison of \( (N) \) and \( (\mathcal{AK}) \): The upsloping and downsloping wedge. We first consider the ASA upsloping wedge underwater acoustic test problem, see [15], with rigid bottom given in the original variables \( r, z \) by the function \( l(r) = 200 - 0.05r \) m for \( 0 \leq r \leq 3339 \) m. The source, of frequency \( f_0 = 25 \) Hz, was placed at \( z_s = 100 \) m and modelled by the initial value \( \psi_0(z) = \sqrt{\frac{\mu_0}{2}} \{\exp(-z - z_s)^2 \frac{k_0^2}{4} - \exp(-(z + z_s)^2 \frac{k_0^2}{4})\} \), \( 0 \leq z \leq l(0) \). 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 \( ik_0 \). The problem was transformed by the change of variables \([1, 0]\) to an equivalent one on the horizontal strip \( 0 \leq x \leq 1, \ 0 \leq t \leq T \), and it was solved numerically by (FE) in both the \( (N) \) and \( (\mathcal{AK}) \) formulations with \( h = 1/1000, \ k = T/1000, \ T = 3339 \). (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 \( \psi \), 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 2 the transmission
loss curves as functions of $r \in [0, 2200 \text{ m}]$ at a depth of $z = 90 \text{ m}$ for both the ($N$) and ($AK$) models, which evidently agree very well.

Figure 2. Upsloping ASA wedge; TL as a function of $r$ at depth $z = 90 \text{ m}$, comparison of ($N$) and ($AK$).

We then considered the analogous downsloping wedge given by $l(r) = 33.05 + 0.05r$ for $0 \leq r \leq 3339 \text{ m}$. The source, of frequency 25 Hz, was placed at $z_s = 25\text{ m}$ and modelled as in the upsloping case. In this case, we found that the (FE) numerical solution of the problem ($N$) apparently exhibited numerical instabilities and did not seem to converge as the discretization parameters became smaller. For example, in Figure 3 we superimpose the TL curves at depth $z = 25\text{ m}$ corresponding to the ($N$) model solved by (FE) with $h = 1/100$, $k = T/100$ and $h = 1/1000$, $k = T/1000$, $T = 3339$, with the analogous results obtained by ($AK$) solved by (FE) with smaller $h$ and $k$. The ($AK$) model, when discretized by (FE), yields reasonable results that converge to the solution shown in Figure 4 with dotted line. To make sure that the numerical method used for ($N$) was not the culprit, we repeated the numerical experiment using a Crank-Nicolson finite difference discretization for ($N$), and found results identical to those of the (FE). We tentatively conclude, therefore, that in this realistic downsloping bottom case, the model ($N$) allows the growth of instabilities, in agreement with the remarks of Abrahamsson and Kreiss in [1] and [2].

Figure 3. Downsloping ASA wedge; TL as a function of $r$ at depth $z = 25\text{ m}$. (FE) solutions for the ($N$) and ($AK$) models.

To check the validity of the ($AK$) solution of this problem we compared the results of Figure 3 with those of yet another numerical method, the Crank-Nicolson type finite difference code IFD for the (PE), [16], [17], [18], which has been widely used in underwater acoustic numerical simulations.
Figure 4. Downsloping ASA wedge; TL as a function of $r$ at a depth $z = 25$ m. Comparison of (N) and (AK), discretized by (FE), and IFD with rigid bottom b.c. (a): $f_0 = 25$ Hz, (b): Magnification of (a) for $r \in [1210, 1430]$, (c): $f_0 = 80$ Hz.

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). Figure 4(a) shows the superimposed TL curves obtained at $z = 25$ m by the (N) and (AK) models solved by (FE) with $h = 1/1000$, $k = T/1000$, $T = 3339$ (as in Figure 3).
and for the IFD with the rigid bottom boundary condition. The results of (AK) and IFD agree well. In fact, they differ by about half a dB as inspection of a typical window of Figure 4(a), shown in Figure 4(b), reveals. (It is worthwhile to note that at a higher frequency \( f_0 = 80 \) Hz the results of (FE)-(AK) and IFD, see Figure 4(c)).

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 \( \psi_r \) term in (PN) by \( \frac{\psi_r}{1 + \sqrt{\psi_r^2 + 4\xi^2}} \) using the (PE), and then discretizing the \( \psi_r \) term at the bottom with one-sided finite differences from the interior of the domain. In the next paragraph 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, (AK) and the rigid bottom boundary condition model implemented by IFD apparently yield correct results, while the Neumann bottom boundary condition used in (N), which retains the term \( \psi_r \) at the bottom, allows the growth of instabilities.

3.3. Using the p.d.e. in the dynamical boundary condition. Let \( w = w(t,y) \) be defined for \( 0 \leq y \leq s(t), \ 0 \leq t \leq T \), and satisfy (1.1)–(1.4). Replace the term \( w_s(t,s(t)) \) in (1.4) by its value given by the p.d.e. in (1.1) to obtain

\[
(3.1) \quad \frac{\partial w}{\partial t}(t,s(t)) - s(t) \left\{ i \frac{1}{2} w_{yy}(t,s(t)) + \left[ i \gamma(t,s(t)) + g(t) \right] w(t,s(t)) \right\} = 0 \quad \forall \ t \in [0,T].
\]

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 \( \tilde{p}(t,y) = w_{yy}(t,y) \). (Note that \( w(t,y) = \int_0^y \tilde{p}(t,\xi) \, d\xi \) since \( w(t,0) = 0 \).) Then, the ibvp (1.1), (1.3), (3.1) becomes

\[
\begin{align*}
\tilde{p}_t & = \frac{1}{2} \tilde{p}_{yy} + i \gamma(t,y) \tilde{p} + i \gamma_y(t,y) w \quad \forall \ y \in [0,s(t)], \ \forall \ t \in [0,T], \\
\tilde{p}(t,0) & = 0 \quad \forall \ t \in [0,T], \\
\tilde{p}(0,y) & = \tilde{p}_0(y) := \psi_0(t) \quad \forall \ y \in [0,0].
\end{align*}
\]

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

In what follows, we shall obtain an \textit{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 \( x := \frac{x}{s(t)} \) that maps the domain of the problem onto the horizontal strip \( \{ (t,x) : t \in [0,T], x \in D \} \), where \( D = (0,1) \). Consider the transformation

\[
(3.3) \quad \tilde{p}(t,y) = \frac{1}{s(t)} \exp(-\zeta(t,x)) \left( p(t,x) - \zeta_x(t,x) \int_0^x p(t,\xi) \, d\xi \right),
\]

where the function \( \zeta \) will be specified below. Note that the function \( \theta \), defined by \( \theta(t,x) := \int_0^x p(t,\xi) \, d\xi \) for \( (t,x) \in [0,T] \times D \), satisfies the first-order o.d.e.

\[
\theta_x(t,x) - \zeta_x(t,x) \theta(t,x) = s(t) \exp(\zeta(t,x)) \tilde{p}(t,x s(t)).
\]

Solving this differential equation with initial condition \( \theta(t,0) = 0 \) yields

\[
\theta(t,x) = s(t) \exp(\zeta(t,x)) \int_0^x \tilde{p}(t,\xi s(t)) \, d\xi,
\]

from which we may derive the inverse of the transformation (3.3) in the form

\[
\begin{align*}
p(t,x) & = s(t) \exp(\zeta(t,x)) \left( \tilde{p}(t,x s(t)) + \zeta_x(t,x) \int_0^x \tilde{p}(t,\xi s(t)) \, d\xi \right). \\
\end{align*}
\]

After some calculations we also obtain that

\[
(3.4) \quad \theta(t,x) = \exp(\zeta(t,x)) w(t,x s(t)), \quad (t,x) \in [0,T] \times D.
\]
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 \( \zeta \), as in [4], by the formula
\[
\zeta(t, x) = \frac{1}{2} \left( \sigma(t) - 1 \right) \dot{s}(t)s(t)x^2 \quad \forall (t, x) \in [0, T] \times \mathcal{D},
\]
where \( \sigma(t) := \frac{2(1+\dot{s}(t)^2)}{s(t)^2} + \varepsilon \), if \( \dot{s}(t) > 0 \), where \( \varepsilon \) is a positive constant, and \( \sigma(t) := 1 \), or equivalently \( \zeta = 0 \), if \( \dot{s}(t) < 0 \). Then, in the transformed domain, and expressed in terms of the new field variables \( p \) and \( \theta \), the ibvp (3.2) becomes
\[
\begin{align*}
\zeta(t, x) &= \frac{1}{2} \left( \sigma(t) - 1 \right) \dot{s}(t)s(t)x^2 \quad \forall (t, x) \in [0, T] \times \mathcal{D}, \\
p_t &= \frac{1}{A(t)} p_{xx} + B(t, x) p_x + \left[ B_x(t, x) + G(t, x) \right] p + G_x(t, x) \theta \quad \forall (t, x) \in [0, T] \times \mathcal{D}, \\
p_x(t, 0) = 0 \quad \forall t \in [0, T], \\
i \frac{1}{A(t)} p_x(t, 1) &= \frac{1-R_1(t)}{R_1(t)} p(t, 1) - \frac{R_1(t)G(t, 1)+R_2(t)}{R_1(t)} \theta(t, 1) \quad \forall t \in [0, T], \\
p(0, x) &= p_0(x) \quad \forall x \in \mathcal{D},
\end{align*}
\]
where \( p_0(x) = \exp(\zeta(0, x)) \left[ w_0'(x) + \zeta_0(x, 0) x \right] \int_0^x w_0'(\xi(0)) d\xi \right], A(t) = 2 s^2(t), R_1(t) = \frac{\dot{s}(t)s(t)}{s(t)^2+\dot{s}(t)^2}, B(t, x) = x \frac{\dot{s}(t)}{s(t)} \zeta(t, x), G(t, x) = \zeta(t, x) - x \frac{\dot{s}(t)}{s(t)} \zeta(t, x) + i \gamma(t, x) \), \( R_2(t) = [g(t) - \zeta(t, 1)] R_1(t) + \zeta(t, 1) \). (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 \( B(t, x) = \frac{\dot{s}(t)s(t)}{s(t)^2+\dot{s}(t)^2} \sigma(t) \), 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 (3.4) is L²-stable.

**Proof.** Multiply the p.d.e. 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
\[
\begin{align*}
\frac{1}{2} \frac{d}{dt} \|p(t, \cdot)\|^2 &= \frac{2-R_1(t)B(t, 1)}{2R_1(t)} \|p(t, 1)\|^2 - \text{Re} \left[ \frac{G(t, 1)R_1(t)+R_2(t)}{R_1(t)} \theta(t, 1) \overline{p(t, 1)} \right] \\
&\quad + \text{Re} \left( G_x(t, \cdot) \theta(t, \cdot), p(t, \cdot) \right) \\
&\quad + \frac{1}{2} \left( B_x(t, \cdot)p(t, \cdot), p(t, \cdot) \right) + \text{Re} \left( G(t, \cdot)p(t, \cdot), p(t, \cdot) \right) \quad \forall t \in [0, T].
\end{align*}
\]
Using the Cauchy-Schwarz inequality, the arithmetic-geometric mean inequality, and noting that \( |\theta(t, 1)| \leq \|p(t, \cdot)\|, |\theta(t, \cdot)| \leq \|p(t, \cdot)\| \) we see from the above that for any \( \lambda > 0 \) there exists a constant \( C_\lambda > 0 \) such that
\[
\frac{d}{dt} \|p(t, \cdot)\|^2 \leq \left( \frac{1}{R_1(t)} - \frac{1}{2} B(t, 1) + \lambda \right) \|p(t, 1)\|^2 + C_\lambda \|p(t, \cdot)\|^2 \quad \forall t \in [0, T].
\]
Since \( \frac{1}{R_1(t)} - \frac{1}{2} B(t, 1) < 0 \) for \( t \in [0, T] \), we may chose \( \lambda \) sufficiently small to make the first term in the right-hand side of the above negative. Hence, by Grönwall’s lemma, we conclude that \( \|p(t, \cdot)\| \leq C \|p_0\| \) for \( t \in [0, T] \), which ends the proof. □

Now, we can define a semiscrete approximation \( p_h : [0, T] \to S_h \) of the solution \( p \) of problem (3.6) by
\[
p_h(0, x) = p_0^h(x) \quad \forall x \in [0, 1],
\]
and
\[
(\partial_t p_h, \phi) = \frac{1}{A(t)} \mathcal{S}(p_h, \phi) + \frac{1-R_1(t)B(t, 1)}{R_1(t)} p_h(t, 1) - \frac{R_1(t)G(t, 1)+R_2(t)}{R_1(t)} \theta_h(t, 1) \phi(1) \\
+ \left( B(t, \cdot) \partial_x p_h, \phi \right) + \left( [B_x(t, \cdot) + G(t, \cdot)] p_h, \phi \right) \\
+ \left( G_x(t, \cdot) \theta_h, \phi \right) \quad \forall \phi \in S_h, \quad \forall t \in [0, T],
\]
where \( \theta_h(t, x) := \int_0^x p_h(t, \xi) d\xi \). We may now prove the following result.

**Theorem 3.1.** If the bottom is strictly monotone, the ibvp (3.4) is L²-stable.
3.4. 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 \( 0 \leq t \leq T \). 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 with the (FE) method up to \( T = 1 \), with \( \beta = f = g = 0 \), \( u_0(x) = -x(x-1)^3 \), \( 0 \leq x \leq 1 \), with mesh parameters \( h = k = 1/500 \), in the case of the eight bottom profiles \( s(t) \), \( 0 \leq t \leq 1 \), labeled (a) to (h) and shown in the left-hand icons of the pairs in Figure 5. (In all cases depth increases downwards.) The right-hand icons show the corresponding, numerically computed, \( L^2 \)-norm of the solution of \( (\mathcal{N}) \) \( ||u(t, \cdot)|| \) for \( 0 \leq t \leq 1 \). (Note that \( ||u(0, \cdot)|| = \frac{1}{6\sqrt{7}} \cong 0.062994 \).) The bottom profiles are given for \( 0 \leq t \leq 1 \) by the 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) \( s(t) = 1 + t^3 \).

Figure 5. Behavior of the \( L^2 \)-norm of the numerical solution of \( (\mathcal{N}) \) as a function of \( t \) for various bottom profiles \( s(t) \).
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 \(t = 1/2\), 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 \(t = 1/2\), 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 \(t > 1/2\). 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 be of course certain about the existence of a singularity at \(t = 1/2\) in the case (g), given that the (FE) code does not at present possess an adaptive refinement capability in \(x\) and \(t\). However, when the experiment was repeated with \(k = h = 1/800\), it was confirmed that the onset of rapid growth occurred at about \(t = 1/2\); 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 re-write here for ease in reading: We seek a real-valued function \(u : [0, T] \times [0, 1] \rightarrow \mathbb{R}\), such that

\[
\begin{align*}
\dot{u}_t &= a(t) u_{xx} + \beta(t, x) u + f(t, x) \quad \forall (t, x) \in [0, T] \times [0, 1], \\
\dot{u}(t, 0) &= 0 \quad \forall t \in [0, T], \\
\dot{u}(t, 1) &= \varepsilon(t) u_t(t, 1) + \delta(t) u(t, 1) + g(t) \quad \forall t \in [0, T], \\
\dot{u}(x, 0) &= u_0(x) \quad \forall x \in [0, 1],
\end{align*}
\]

(4.1)

where \(\beta : [0, T] \times [0, 1] \rightarrow \mathbb{R}, f : [0, T] \times [0, 1] \rightarrow \mathbb{R}, \delta : [0, T] \rightarrow \mathbb{R}, g : [0, T] \rightarrow \mathbb{R}, a : [0, T] \rightarrow (0, +\infty)\) with \(a_* := \inf_{[0, T]} a > 0, \varepsilon : [0, T] \rightarrow \mathbb{R}, u_0 : [0, 1] \rightarrow \mathbb{R}, \) 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 \(\varepsilon\).

4.1. The dissipative case. The dissipative case is characterized by the assumption \(\varepsilon(t) \leq 0\) for \(t \in [0, T]\); the problem is well posed, see e.g. \([14]\). 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 Section \(2.1\) restricting ourselves to the real case, and avoiding the inverse inequality \((2.5)\).

4.1.1. Semidiscrete approximation. Find \(u_h : [0, T] \rightarrow S_h\), a space-discrete approximation of \(u\), requiring

\[
(\partial_t u_h(t, \cdot), \chi) = \left[ \varepsilon(t) \partial_t u_h(t, 1) + \delta(t) u_h(t, 1) + g(t) \right] \chi(1)
- a(t) \mathcal{B}(u_h(t, \cdot), \chi) + (\beta(t, \cdot) u_h(t, \cdot), \chi) + (f(t, \cdot), \chi) \quad \forall \chi \in S_h, \quad \forall t \in [0, T],
\]

(4.2)

and

\[
\dot{u}_h(0, \cdot) = R_h u_0(\cdot).
\]

Proposition 4.1. If \(\varepsilon \leq 0\), then the problem \((4.2)\) admits a unique solution \(u_h \in C^1([0, T]; S_h)\).

\textit{Proof.} The result follows if we argue along the lines of the proof of Proposition \((2.3)\) \(\square\)

Proposition 4.2. Let \(u\) be the solution of \((4.1)\) and \(u_h\) its semidiscrete approximation defined by \((4.2)\). If \(\varepsilon(t) \leq 0\) for \(t \in [0, T]\), then

\[
\|u_h(t, \cdot) - R_h u(t, \cdot)\|_h^2 \leq C h^{2(r+1)} \left( \int_0^t \Gamma_D(\tau) d\tau \right) \quad \forall t \in [0, T], \quad \forall h \in (0, h_*],
\]

(4.4)

where \(\Gamma_D(\tau) := \|u(\tau, \cdot)\|_{r+1}^2 + \|\partial_t u(\tau, \cdot)\|_{r+1}^2\).
Proof. Let \( h \in (0, \bar{h}] \) and \( \theta_h := u_h - R_h u \). Using (4.2), the p.d.e. in (4.1), (2.3) and (2.8) we obtain

\[
(\partial_t \theta_h(t, \cdot), \chi) = [\varepsilon(t) \partial_t \theta_h(t, 1) + \delta(t) \theta_h(t, 1)] \chi(1) - a(t) B(\theta_h(t, \cdot), \chi) \\
+ (\beta(t, \cdot) \theta_h(t, \cdot), \chi) + (\Phi_*(t, \cdot), \chi) \quad \forall \chi \in S_h, \quad \forall t \in [0, T],
\]

where \( \Phi_* := [\partial_t u - R_h(\partial_t u)] - \beta(u - R_h u) \). First we observe that from (4.2) it follows that

\[
\|\Phi_*(t, \cdot)\| \leq C h^{r+1} \left[ \|u(t, \cdot)\|_{r+1} + \|\partial_t u(t, \cdot)\|_{r+1} \right] \quad \forall t \in [0, T].
\]

Setting \( \chi = \theta_h \) in (4.5) and using (2.3), we obtain

\[
\frac{d}{dt} \|\theta_h(t, \cdot)\|^2 \leq \frac{|\varepsilon(t)|}{c} |\partial_t \theta_h(t, 1)|^2 - 2a_*|\theta_h(t, \cdot)|^2 \\
+ 2 \|\Phi_*(t, \cdot)\| \|\theta_h(t, \cdot)\| + 2 \max_{[0,1]} |\beta(t, \cdot)| \|\theta_h(t, \cdot)\|^2 \\
+ 2 \|\Phi_*(t, \cdot)\| \|\partial_t \theta_h(t, \cdot)\| \|\theta_h(t, \cdot)\|_1 \quad \forall t \in [0, T], \quad \forall \varepsilon > 0,
\]

which, along with (4.6), yields

\[
\frac{d}{dt} \|\theta_h(t, \cdot)\|^2 \leq |\varepsilon(t)| |\partial_t \theta_h(t, 1)|^2 + C (\varepsilon + \varepsilon^3) \|\theta_h(t, \cdot)\|^2 + \varepsilon h^{2(r+1)} \Gamma_D(t) \quad \forall t \in [0, T], \quad \forall \varepsilon > 0.
\]

Set \( \chi = \partial_t \theta_h \) in (4.5) to obtain

\[
\frac{d}{dt} \left[ a(t) \|\theta_h(t, \cdot)\|^2 - \delta(t) |\theta_h(t, 1)|^2 \right] = -2 |\varepsilon(t)| |\partial_t \theta_h(t, 1)|^2 - \delta(t) |\theta_h(t, 1)|^2 \\
+ \dot{a}(t) |\theta_h(t, \cdot)|^2 - 2 |\partial_t \theta_h(t, \cdot)|^2 \\
+ 2 (\beta(t, \cdot) \theta_h(t, \cdot), \partial_t \theta_h(t, \cdot)) + 2 (\Phi_*(t, \cdot), \partial_t \theta_h(t, \cdot)) \quad \forall t \in [0, T],
\]

which, in view of (2.3) and (4.6), yields that

\[
\frac{d}{dt} \left[ a(t) \|\theta_h(t, \cdot)\|^2 - \delta(t) |\theta_h(t, 1)|^2 \right] \leq -2 |\varepsilon(t)| |\partial_t \theta_h(t, 1)|^2 + C \|\theta_h(t, \cdot)\|^2 + \varepsilon h^{2(r+1)} \Gamma_D(t) \quad \forall t \in [0, T].
\]

For positive \( \varepsilon \) we define

\[
\nu_\varepsilon(t) := \varepsilon \|\theta_h(t, \cdot)\|^2 + a(t) |\theta_h(t, \cdot)|^2 - \delta(t) |\theta_h(t, 1)|^2 \quad \forall t \in [0, T].
\]

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

\[
\nu_\varepsilon(t) \geq \varepsilon \|\theta_h(t, \cdot)\|^2 + a_* |\theta_h(t, \cdot)|^2 - 2|\delta(t)| \|\theta_h(t, \cdot)\| \|\theta_h(t, \cdot)\|_1 \\
\geq \frac{\varepsilon}{2} |\theta_h(t, \cdot)|^2 + \left( \varepsilon - \frac{2|\delta(t)|^2}{a_*} \right) \|\theta_h(t, \cdot)\|^2 \quad \forall t \in [0, T].
\]

If \( \varepsilon_0 := \frac{\varepsilon}{2} + \frac{2}{a_*} \max_{[0,T]} |\theta|^2 \), (4.10) yields that

\[
\nu_{\varepsilon_0}(t) \geq \frac{\varepsilon}{2} \|\theta_h(t, \cdot)\|^2 \quad \forall t \in [0, T].
\]

Now, setting \( \varepsilon = \varepsilon_0 \) in (4.7) and then adding the resulting equation with (4.3), we obtain

\[
\dot{\nu}_{\varepsilon_0}(t) \leq C \nu_{\varepsilon_0}(t) + (\varepsilon_0 + 1) h^{2(r+1)} \Gamma_D(t) \quad \forall t \in [0, T].
\]

Since \( \theta_h(0, \cdot) = 0 \), the bound (4.4) follows from (4.12) via Grönwall’s lemma and (4.11). □

A simple consequence of (2.7) and (4.3) is the following optimal-order error estimate.

**Theorem 4.3.** Let \( u \) be the solution of (4.1) and \( u_h \) its semidiscrete approximation defined by (4.2) and (4.3). If \( \varepsilon(t) \leq 0 \) for \( t \in [0, T] \), then

\[
\|u_h(t, \cdot) - u(t, \cdot)\| + h \|u_h(t, \cdot) - u(t, \cdot)\|_1 \leq C h^{r+1} \left[ \|u(t, \cdot)\|_{r+1} + \left( \int_0^t \Gamma_D(\tau) d\tau \right)^{1/2} \right] \quad \forall t \in [0, T],
\]

where \( \Gamma_D \) is the function defined in the statement of Proposition 4.2. □
4.1.2. Crank-Nicolson fully discrete approximations. We use the notation of paragraph 2.2.2. For \( n = 0, \ldots, N \), the Crank-Nicolson method for the problem (1.1) yields an approximation \( U^n_h \in S_h \) of \( u(t^n, \cdot) \) as follows:

**Step 1:** Set

\[
(4.14) \quad U^0_h := R_h u_0.
\]

**Step 2:** For \( n = 1, \ldots, N \), find \( U^n_h \in S_h \) such that

\[
(4.15) \quad (\partial U^n_h, \chi) = \left[ \varepsilon_n^{-\frac{1}{2}} \partial U^n_h(1) + \delta_n^{-\frac{1}{2}} AU^n_h(1) + g_n^{-\frac{1}{2}} \right] \chi(1)
\]

\[
- a_n^{-\frac{1}{2}} B(AU^n_h, \chi) + (\beta_n^{-\frac{1}{2}} AU^n_h, \chi) + (f_n^{-\frac{1}{2}}, \chi) \quad \forall \chi \in S_h,
\]

where \( a_n^{-\frac{1}{2}} := a(t_n^{-\frac{1}{2}}) \), \( \delta_n^{-\frac{1}{2}} := \delta(t_n^{-\frac{1}{2}}) \), \( \varepsilon_n^{-\frac{1}{2}} := \varepsilon(t_n^{-\frac{1}{2}}) \), \( g_n^{-\frac{1}{2}} := g(t_n^{-\frac{1}{2}}) \), \( f_n^{-\frac{1}{2}} := f(t_n^{-\frac{1}{2}}) \) and 

\[
\beta_n^{-\frac{1}{2}} := \beta(t_n^{-\frac{1}{2}}, \cdot).
\]

**Proposition 4.4.** Let \( n \in \{1, \ldots, N\} \) and suppose that \( U^{n-1}_h \in S_h \) is well defined. If \( \varepsilon_n^{-\frac{1}{2}} \leq 0 \), then there exists a constant \( C_n \) such that if \( k_n < C_n \), then \( U^n_h \) is well defined by (1.15).

**Proof.** It is easy to show that if there is a \( V \in S_h \) such that

\[
(4.16) \quad \frac{1}{k_n} (V, \phi) = \left[ \frac{\varepsilon_n^{-\frac{1}{2}}}{k_n} V(1) + \frac{\delta_n^{-\frac{1}{2}}}{2} V(1) \right] \phi(1) - \frac{\varepsilon_n^{-\frac{1}{2}}}{2} B(V, \phi) + \frac{1}{2} (\beta_n^{-\frac{1}{2}} V, \phi) \quad \forall \phi \in S_h,
\]

then \( V = 0 \). To arrive at the desired conclusion, first set \( \phi = V \) in (4.10) and use (2.3) to obtain

\[
\|V\|^2 + \|\varepsilon_n^{-\frac{1}{2}}\| |V(1)|^2 \leq \frac{\varepsilon_n}{2} \left( 2\|\delta_n^{-\frac{1}{2}}\| \|V\| + \|\beta_n^{-\frac{1}{2}}\| \|V\|^2 \right).
\]

Then use the arithmetic-geometric mean inequality, to get

\[
\|V\|^2 (1 - k_n \gamma_n) \leq 0,
\]

where \( \gamma_n = \frac{1}{2} \left( |\beta_n^{-\frac{1}{2}}|_{\infty} + \frac{|\varepsilon_n^{-\frac{1}{2}}|_{\infty}^2}{\frac{1}{2}} \right) \). This yields \( V = 0 \) if we require, for example, \( k_n < \frac{1}{1 + \gamma_n} \). □

The following consistency result is analogous to that of Proposition 2.8.

**Proposition 4.5.** Let \( u \) be the solution of (1.1). For \( n = 1, \ldots, N \), define \( \sigma^n : D \to \mathbb{R} \) by

\[
(4.17) \quad a_n^{-\frac{1}{2}} u_{x x}(t_n^{-\frac{1}{2}}, \cdot) + \beta_n^{-\frac{1}{2}} A u^n + f^n = \sigma^n.
\]

Then

\[
(4.18) \quad \|\sigma^n\| \leq C(k_n)^2 \left( \max_{|n-\ell| \leq n} \|\partial^2 u\| + \max_{|n-\ell| \leq n} \|\partial^3 u\| \right), \quad n = 1, \ldots, N. \quad □
\]

**Proposition 4.6.** Let \( u \) be the solution of (1.1) and \( (U^n_h)_{n=0}^N \) be the fully discrete approximations that the method of (4.14)-(1.15) produces. Assume that \( \varepsilon(t) \leq 0 \) for \( t \in [0, T] \), and that (2.22) holds. Then, there exists a constant \( C_D \geq 0 \) such that: if \( \max_{1 \leq n \leq N} \|U^n_h - R_h u^n\|_1 \leq \frac{1}{3}, \) there exists a constant \( C > 0 \) such that

\[
(4.19) \quad \max_{1 \leq n \leq N} \|U^n_h - R_h u^n\|_1 \leq C \left( k^2 + h^{r+1} \right) \chi_D(u) \quad \forall u \in (0, h),
\]

where \( \chi_D(u) := \sum_{\ell=1}^4 \max_{|\ell| \\leq n} \|\partial^\ell u\|_{r+1} + \sum_{\ell=2}^4 \max_{|\ell| \\leq n} \|\partial^\ell u\|_1 + \sum_{\ell=2}^4 \max_{|\ell| \\leq n} \|\partial^\ell u(t, 1)\| \).

**Proof.** Let \( h \in (0, h_n] \), \( \delta_n := \delta(t^n) \), \( a_n := a(t^n) \) and \( \theta^n_h := U^n_h - R_h u^n \) for \( n = 0, \ldots, N \). We use (4.15), (4.17), (2.6), and (2.3), to obtain

\[
(4.20) \quad (\partial \theta^n_h, \chi) = \left[ \varepsilon_n^{-\frac{1}{2}} \partial \theta^n_h(1) + \delta_n^{-\frac{1}{2}} A \theta^n_h(1) - Z^n_3 \right] \chi(1) - a_n^{-\frac{1}{2}} B(A \theta^n_h, \chi) + (\beta_n^{-\frac{1}{2}} A \theta^n_h, \chi)
\]

\[
+ (Z^n_1 - a_n \chi) + a_n^{-\frac{1}{2}} B(Z^n_2, \chi) \quad \forall \chi \in S_h, \quad n = 1, \ldots, N,
\]
where $Z_n^1 := \partial u^n - R_h(\partial u^n) - P_h[\beta a^{n-\frac{1}{2}} (Au^n - R_h(Au^n))]$, $Z_n^2 := u(t^n - \frac{1}{2}) - Au^n$ and $Z_n^3 := \varepsilon^{n-\frac{1}{2}} \left[ \partial u(t^n - \frac{1}{2}, 1) - \partial u^n(1) \right] + \delta^{n-\frac{1}{2}} \left[ u(t^n - \frac{1}{2}) - Au^n(1) \right]$. Using Taylor's formula and (2.7), we deduce the following estimates:

\begin{align}
\|Z_n^1\| &\leq C h^{r+1} \left[ \max_{[\delta^{-1}, \varepsilon^{-1}]} \|u\|_{r+1} + \max_{[\delta^{-1}, r^{-1}]} \|\partial_t u\|_{r+1} \right], \\
|Z_n^2| &\leq C k_n^2 \max_{[\delta^{-1}, \varepsilon^{-1}]} |\partial_t^2 u|_1, \\
|Z_n^3| &\leq C k_n^2 \left[ \max_{t \in [\varepsilon^{-1}, \delta^{-1}]} |\partial_t^3 u(t, 1)| + \max_{t \in [\varepsilon^{-1}, \delta^{-1}]} |\partial_t^2 u(t, 1)| \right],
\end{align}

for $n = 1, \ldots, N$. The proof now proceeds in four steps.

**Step I:** Set $\chi = A\theta_h^n$ in (120) and use (2.3) and the Cauchy-Schwarz inequality, to obtain

\begin{align}
\|\theta_h^n\|^2 + |\varepsilon^n| |\theta_h^n(1)|^2 &\leq |\theta_h^{n-1}|^2 + |\varepsilon^{n-1}| |\theta_h^{n-1}(1)|^2 \\
&+ (\varepsilon^{n-\frac{1}{2}} - \varepsilon^n) |\theta_h^n(1)|^2 + (\varepsilon^{n-1} - \varepsilon^{n-\frac{1}{2}}) |\theta_h^{n-1}(1)|^2 \\
&+ 2k_n \left[ (\sigma^n \cdot \frac{a}{a^n}) |A\theta_h^n| \|A\theta_h^n\|_1 - a \cdot |A\theta_h^n|^2 + \|\beta_a^{n-\frac{1}{2}}\|_\infty \|A\theta_h^n\|^2 \\n&+ \sqrt Z_n^a \|A\theta_h^n\|^{\frac{1}{2}} |A\theta_h^n| \|A\theta_h^n\|_1 \|A\theta_h^n\|_1 \right] \\
&+ (|\sigma^n| + \|Z_n^1\|) \|A\theta_h^n\| + a^{n-\frac{1}{2}} |Z_n^2|_1 |A\theta_h^n|_1, \quad n = 1, \ldots, N,
\end{align}

which, after the use of the arithmetic-geometric mean inequality, yields

\begin{align}
\|\theta_h^n\|^2 + |\varepsilon^n| |\theta_h^n(1)|^2 &\leq |\theta_h^{n-1}|^2 + |\varepsilon^{n-1}| |\theta_h^{n-1}(1)|^2 + C k_n \left( |\theta_h^n(1)|^2 + |\theta_h^{n-1}(1)|^2 \right) \\
&+ C k_n \left( |\theta_h^n| \|A\theta_h^n\| + \|\sigma^n\| \|A\theta_h^n\| + \|\beta_a^{n-\frac{1}{2}}\|_\infty \|A\theta_h^n\|^2 \right) \\
&+ |\sigma^n| + \|Z_n^1\| + \|Z_n^2\|_1 + \|Z_n^3\|_1, \quad n = 1, \ldots, N.
\end{align}

**Step II:** Now set $\chi = \theta_h^n$ in (420) to get

\begin{align}
|\theta_h^n|^2 - \frac{\sigma_n}{a^n} |\theta_h^n(1)|^2 &\leq |\theta_h^{n-1}|^2 - \frac{\delta^n}{a^{n-1}} |\theta_h^{n-1}(1)|^2 - 2k_n \left( |\theta_h^n|^2 + \|\beta_a^{n-\frac{1}{2}}\|_\infty \|A\theta_h^n\| \|A\theta_h^n\| + a^{n-\frac{1}{2}} |B(Z_n^a, \theta_h^n)\| \right) \\
&+ \left( - \frac{\delta^n}{a^{n-\frac{1}{2}}} - \frac{\delta^n}{a^n} \right) |\theta_h^n(1)|^2 + \left( - \frac{\delta^n}{a^{n-\frac{1}{2}}} + \frac{\delta^n}{a^n} \right) |\theta_h^{n-1}(1)|^2, \quad n = 1, \ldots, N,
\end{align}

which, after the use of the arithmetic-geometric mean inequality, yields

\begin{align}
|\theta_h^n|^2 - \frac{\sigma_n}{a^n} |\theta_h^n(1)|^2 &\leq |\theta_h^{n-1}|^2 - \frac{\delta^n}{a^{n-1}} |\theta_h^{n-1}(1)|^2 + C k_n \left( |\theta_h^n(1)|^2 + |\theta_h^{n-1}(1)|^2 \right) \\
&+ 2k_n \left( |B(Z_n^a, \theta_h^n)| + \frac{1}{a^{n-\frac{1}{2}}} |Z_n^2| \|\theta_h^n(1)\| \right) \\
&+ C k_n \left( \|\theta_h^n| \|A\theta_h^n\| + \|\theta_h^{n-1}\| \|A\theta_h^n\| + \|\theta_h^n\|_1 \|A\theta_h^n\|_1 \right), \quad n = 1, \ldots, N.
\end{align}

**Step III:** For $\rho > 0$, we introduce the quantities

\begin{align}
\nu_h^m := \rho \left( \|\theta_h^n\|^2 + |\varepsilon^n| |\theta_h^n(1)|^2 \right) + |\theta_h^n|^2 - \frac{\delta^n}{a^{n-1}} |\theta_h^n(1)|^2, \quad m = 0, \ldots, N.
\end{align}

Now, using (4.26) and (2.3) we have

\begin{align}
\nu_h^m &\geq \rho \|\theta_h^n\|^2 + |\theta_h^n|^2 \left( - \frac{\delta^n}{a^{n-1}} \right), \quad m = 0, \ldots, N.
\end{align}
Thus, choosing $\rho = \rho_0 := \frac{1}{2} + 2 \max_{[0,T]} \frac{\Delta^2}{\Delta t}$, we obtain

$$\mathcal{V}_\rho^m \geq \frac{1}{2} \|\theta_k^m\|_1^2, \quad m = 0, \ldots, N.$$  

(4.27)

**Step IV:** Combining (4.24), (4.26), (4.28), (4.29), (4.30), and (4.31) we obtain

$$\mathcal{V}_\rho^m \leq \mathcal{V}_{\rho_0}^{m-1} + C K_n \left( \|\theta_k^m\|_1^2 + \|\theta_k^{m-1}\|_1^2 \right) + C K_n \left[ (k_n)^2 + (h^{r+1})^2 \right] (\Upsilon_1(u))^2 + 2 K_n \left[ B(Z_n^2, \partial \theta_k^m) - \frac{1}{a_n - \frac{2}{3}} Z_n^2 \partial \theta_k^m(1) \right], \quad n = 1, \ldots, N,$$

where $\Upsilon_1(u) := \max_{[0,T]} \|u\|_{r+1} + \max_{[0,T]} \|\partial u\|_{r+1} + \max_{[0,T]} \|\emptyset^2 u\|_1 + \max_{[0,T]} \|\emptyset^2 u\|_1 + \max_{l=1}^{m-1} |\emptyset^2 u_l(1)| + \max_{l=1}^{m-1} |\emptyset^2 u_l(1)|$. Using (4.28) and (4.29) we conclude that there exist constants $C_1 \geq 0$ and $C_2 \geq 0$, such that

$$(1 - C_1 K_n) \mathcal{V}_\rho^m \leq (1 + C_1 K_n) \mathcal{V}_{\rho_0}^{m-1} + C_2 K_n (h^{r+1} + k_n^2) (\Upsilon_1(u))^2 + 2 K_n \left[ B(Z_n^2, \partial \theta_k^m) - \frac{1}{a_n - \frac{2}{3}} Z_n^2 \partial \theta_k^m(1) \right], \quad n = 1, \ldots, N.$$  

(4.29)

To continue, we assume that $\max_{1 \leq n \leq N} (C_1 K_n) \leq \frac{1}{3}$, which allows us to conclude that $C_2 K_n \leq e^{3C_1 K_n}$ for $n = 1, \ldots, N$. Hence, (4.29) yields

$$\mathcal{V}_\rho^m \leq e^{3C_1 K_n} \mathcal{V}_{\rho_0}^{m-1} + C_2 K_n (h^{r+1} + k_n^2) (\Upsilon_1(u))^2 + 2 K_n \left[ B(Z_n^2, \partial \theta_k^m) - \frac{1}{a_n - \frac{2}{3}} Z_n^2 \partial \theta_k^m(1) \right], \quad n = 1, \ldots, N.$$  

Letting $\lambda_j^m := \frac{\exp(3C_1 \sum_{k_j=1}^n k_j)}{1 - C_1 K_n}$ and using a simple inducti argument we arrive at

$$\mathcal{V}_\rho^m \leq C_2 (\Upsilon_1(u))^2 \sum_{j=1}^n k_j \lambda_j^m (h^{r+1} + k_n^2)^2 + 2 \sum_{j=1}^n k_j \lambda_j^m \left[ B(Z_n^2, \partial \theta_k^m) - \frac{1}{a_n - \frac{2}{3}} Z_n^2 \partial \theta_k^m(1) \right], \quad n = 1, \ldots, N,$$

which yields

$$\mathcal{V}_\rho^m \leq C (h^{r+1} + k_n^2)^2 (\Upsilon_1(u))^2 + T_2^m + T_1^m, \quad n = 1, \ldots, N,$$

where $T_1^m := 2 \sum_{j=1}^n \lambda_j^m B(Z_n^2, \theta_j^m - \theta_j^{m-1})$ and $T_2^m := -2 \sum_{j=1}^n \frac{\lambda_j^m}{a_n - \frac{2}{3}} Z_n^2 (\theta_j^m(1) - \theta_j^{m-1}(1))$. First, we proceed as in bounding the quantity $T_1^m$ in the proof of Proposition (2.7.9) to get

$$|T_1^m| \leq C k^2 \Upsilon_2(u) \max_{1 \leq m \leq n} |\theta_k^m|_1, \quad n = 1, \ldots, N,$$

where $\Upsilon_2(u) := \max_{[0,T]} \|\emptyset^2 u\|_1 + \max_{[0,T]} \|\emptyset^2 u\|_1$. In addition, we have

$$-T_2^m = \frac{2}{1 - C_1 K_n} \frac{1}{a_n - \frac{2}{3}} Z_n^2 \theta_k^m(1) + \frac{n-1}{2} \sum_{j=1}^{n-1} \frac{\lambda_j^m}{a_n - \frac{2}{3}} \left( Z_n^2 - Z_n^{j+1} \right) \theta_j^{j+1}(1) + 2 \sum_{j=1}^{n-1} \exp(3C_1 \sum_{k_j=1}^n k_j) \left[ \exp(3C_1 \sum_{k_{j+1}=1}^n k_{j+1}) - \frac{C_1 k_{j+1}}{1 - C_1 k_{j+1}} \right] Z_n^{j+1} \theta_j^{j+1}(1) + 2 \sum_{j=1}^{n-1} \left( \frac{1}{a_n - \frac{2}{3}} - \frac{1}{a_n + \frac{2}{3}} \right) \lambda_j^{j+1} Z_n^{j+1} \theta_j^{j+1}(1), \quad n = 1, \ldots, N.$$  

(4.32)

Observing that

$$|Z_n^2 - Z_n^{j+1}| \leq C (k_j + k_{j+1}) \left[ (k_j)^2 + \|k_j - k_{j+1}\| \right] \Upsilon_3(u), \quad j = 1, \ldots, N - 1,$$

with $\Upsilon_3(u) := \sum_{l=2}^4 \max_{t \in [0,T]} |\emptyset^l u_l(t,1)|$, we see that (4.32), (4.28), (4.29) and (4.31) yield
Theorem 4.7. Let
\[ (4.14) \]
method (4.14) which is the desired estimate (4.19).
\[ \square \]

Now, from (4.30), (4.31) and (4.33) there follows that
\[ \text{Use then (4.27) to arrive at} \]
\[ \max_{0 \leq n \leq N} \| \theta_n^m \|_1^2 \leq C (h^{r+1} + k^2) (\mathcal{Y}_1(u) + \mathcal{T}_2(u) + \mathcal{Y}_3(u))^2, \]
which is the desired estimate (4.19).
\[ \square \]

As a simple consequence of (4.19) and (2.7) we obtain the following optimal-order error estimates in \( L^2 \) and \( H^1 \) norms.

**Theorem 4.7.** Let \( u \) be the solution of (4.1) and \( (U^m_n)^{n=0} \) be the fully discrete approximations that the method (4.14)–(4.17) produces. Assume that \( \varepsilon(t) \leq 0 \) for \( t \in [0, T] \), that (2.28) holds and \( \max_{1 \leq n \leq N} C_\nu C_D \leq \frac{1}{2} \), where \( C_\nu \) is the constant specified in Proposition 4.6. Then
\[ \max_{0 \leq n \leq N} \| U^m_n - u^m \|_\varepsilon \leq C (k^2 + h^{r+1-\ell}) \mathcal{Y}_\nu(u), \quad \forall \ h \in (0, h_*], \]
for \( \ell = 0, 1 \), where \( \mathcal{Y}_\nu(u) \) was specified in Proposition 4.6.
\[ \square \]

4.2. The reactive case. In this paragraph, we propose finite element approximations when the dynamical boundary condition in (4.1) is of reactive type, i.e. \( \varepsilon(t) > 0 \) for \( t \in [0, T] \). According to [24], [7], the problem is well posed only in the one-dimensional case. To construct a finite element method for this problem we follow the idea (cf. paragraph 3.3) to replace the term \( u_t \) in the dynamical boundary condition using the partial differential equation in (4.1). Hence we obtain:
\[ a(t) u_{xx}(t, 1) = \frac{\alpha(t)}{\varepsilon(t)} v_x(t, 1) - \frac{\beta(t)}{\varepsilon(t)} v(t, 1) + f(t, 1) \]
for \( t \in [0, T] \). Then, to use this as a boundary condition, we formulate a variational formulation using \( B(\cdot, \cdot) \) instead of the \( L^2(D) \) inner product \( (\cdot, \cdot) \). Of course this approach works also if \( \varepsilon(t) < 0 \) for \( t \in [0, T] \).

4.2.1. Preliminaries. Let \( r \in \mathbb{N} \) with \( r \geq 3 \), and \( S_h \) be a finite-dimensional subspace of \( H^2(D) \) consisting of \( C^1 \) functions that are polynomials of degree less or equal to \( r \) in each interval of a non-uniform partition of \( D \) with maximum length \( h \in (0, h_*] \). It is well-known, [9], that the following approximation property holds:
\[ \inf_{\chi \in S_h} \| v - \chi \|_2 \leq C h^{s-1} \| v \|_{s+1}, \quad \forall v \in H^{s+1}(D), \quad \forall h \in (0, h_*], \quad s = 1, \ldots, r. \]

We introduce bilinear forms \( B^*, \gamma^* : H^2(D) \times H^2(D) \to \mathbb{R} \) given by \( B^*(v, w) := (v'', w'') \) and \( \gamma^*(v, w) := (v''', w''') + (v', w') \) 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 \( R^*_h : H^2(D) \to S_h \) by
\[ \gamma^*(R^*_h v, v) = \gamma^*(v, v) \quad \forall v \in S_h. \]

**Lemma 4.8.** The elliptic projection \( R^*_h \) has the following property
\[ (R^*_h v)'(1) = v'(1) + (R^*_h v - v)(1) - \frac{1}{4} B(R^*_h v - v, \omega) \quad \forall v \in H^2(D), \]
where \( \omega(x) = x^3 \).

**Proof.** Let \( v \in H^2(D) \) and \( \rho = R^*_h v - v \). Since \( \omega \in S_h \), setting \( \chi = \omega \) in (4.33) we obtain
\[ \int_D \rho''(x) x \, dx = -\frac{1}{6} (\rho', \omega'). \]
Then, integrating by parts we get \( \rho'(1) = \rho(1) - \rho(0) - \frac{1}{3} (\rho', \omega') \), which is the desired equality, since \( \rho(0) = 0 \). \( \square \)
Proposition 4.9. The elliptic projection $R_h^s$ has the following approximation properties:

\[
\sum_{\ell=1}^{2} h^\ell \| R_h^s v - v \|^\ell \leq C h^{s+1} \| v \|_{s+1}
\]

and

\[
| (R_h^s v - v)'(1) | + | (R_h^s v - v)(1) | \leq C h^s \| v \|_{s+1}
\]

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

Proof. Let $h \in (0, h_*]$, $s \in \{1, \ldots, r\}$, $v \in \mathbb{H}^{s+1}(D)$ and $e = R_h^s v - v$. Using (4.35) we have $\gamma^s(e, e) = \gamma^s(e, v) - \gamma^s(e, v) - \gamma^s(v, v) - \gamma^s(v, v)$ for $\chi \in S_h$, which along with (4.34) yields

\[
| e |_2 + | e |_1 \leq C h^{s-1} \| v \|_{s+1}.
\]

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

\[
-w'''' + w' = e' \quad \text{in } D,
\]

\[
w(0) = w'(0) = w''(0) = 0.
\]

It is easily seen that (4.40) 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

\[
\| w \|_3 \leq C | e |_1.
\]

Thus, we obtain $\| e' \|_3 = \gamma^s(e, w - \chi)$ for $\chi \in S_h$. Then, we use (4.39), (4.34) and (4.41) to get

\[
| e |^2 \leq C ( | e |_2 + | e |_1 ) h^3 \| w \|_3 \leq C h^s \| v \|_{s+1} \| e |_1,
\]

which yields

\[
| e |_1 \leq C h^s \| v \|_{s+1}.
\]

Hence, (4.37) follows as a simple consequence of (4.39) and (4.42).

Using (4.36), (2.3), (2.1), and (4.37) we have

\[
| e'(1) |^2 + | e(1) |^2 \leq C \left( | e(1) |^2 + \| e' \|_2^2 \right) \leq C | e |^2 \leq C h^{2s} \| v \|_{s+1}^2,
\]

which obviously yields (4.38). □

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

Lemma 4.10. For $v \in H^2(D)$ it holds that

\[
| v'(1) |^2 \leq | v |^2 + 2 | v |_1 | v |_2.
\]

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 (4.43) via the Cauchy-Schwarz inequality. □

4.2.2. Semidiscrete approximation. We define $u_h : [0, T] \to S_h$, a space-discrete approximation of $u$, requiring

\[
B(\partial_t u_h(t, \cdot), \chi) = \left\{ \mathcal{a}(t) \partial_t u_h(t, 1) - \left[ \mathcal{b}(t) + \beta(t, 1) \right] u_h(t, 1) - \left[ \mathcal{d}(t) + f(t, 1) \right] \right\} \chi'(1)
\]

\[
+ f(t, 0) \chi'(0) - \mathcal{a}(0) B^*(u_h(t, \cdot), \chi)
\]

\[
+ B(\beta(t, \cdot) u_h(t, \cdot), \chi) + B(f(t, \cdot), \chi) \ \forall \chi \in S_h, \ \forall t \in [0, T],
\]

and

\[
u_h(0, \cdot) = R_h^s u_0(\cdot).
\]

Proposition 4.11. If $\varepsilon(t) > 0$ for $t \in [0, T]$, then the problem (4.44)-(4.45) admits a unique solution $u_h \in C^1([0, T]; S_h)$. 

Proof. The result follows if we argue along the lines of the proof of Proposition [2.3].

In the sequel, we assume that the solution of the ibvp (4.1) in the reactive case is sufficiently smooth.

**Theorem 4.12.** Let $u$ be the solution of (4.1), $u_h$ its semidiscrete approximation defined by (4.44)-(4.45), and $\Gamma_\theta$ be the function specified in Proposition 4.2. If $\varepsilon > 0$ for $t \in [0, T]$, then

\[(4.46) \quad \|u_h(t, \cdot) - u(t, \cdot)\|_1 \leq C h^{r'} \left[ \|u(t, \cdot)\|_{r+1} + \left( \int_0^t \Gamma_\theta(\tau) \, d\tau \right)^{\frac{r}{r+1}} \right] \quad \forall t \in [0, T], \ \forall h \in (0, h_*].\]

**Proof.** Let $h \in (0, h_*]$, $\theta_h := u_h - R_h^1 u$, and $\eta = R_h^1 u - u$. Using (4.44), (4.35) and (4.1), we obtain

\[(4.47) \quad B(\partial_t \theta_h(t, \cdot), \chi) = \left\{ \frac{a(t)}{\varepsilon(t)} \partial_x \theta_h(t, 1) - \frac{\delta(t)}{\varepsilon(t)} + \beta(t, 1) \right\} \theta_h(t, 1) + \mathcal{E}_{n,2}(t) \chi'(1)
\]

\[\quad - a(t) B^*(\theta_h(t, \cdot), \chi) + B(\beta(t, \cdot) \theta_h(t, \cdot), \chi) \]

\[\quad + B(\mathcal{E}_{n,1}(t, \cdot), \chi) + a(t) \mathcal{E}_{n,2}(t) u(t, \cdot) \]

where $\mathcal{E}_{n,1} := [\partial_t u - R_h^1(\partial_t u)] - \beta(t - u - R_h^1 u)$ and $\mathcal{E}_{n,2}(t) := \frac{a(t)}{\varepsilon(t)} \partial_x \eta(1) - \left[ \frac{\delta(t)}{\varepsilon(t)} + \beta(t, 1) \right] \eta(t, 1)$. First observe that using (4.37), (4.38), and (2.1), it follows that

\[(4.48) \quad |B(\mathcal{E}_{n,1}(t, \cdot), \chi) + a(t) \mathcal{E}_{n,2}(t) u(t, \cdot)| \leq C h^{r'} \left( \|u(t, \cdot)\|_{r+1} + \|\partial_t u(t, \cdot)\|_{r+1} \right) |\chi(1)|\]

and

\[(4.49) \quad |\mathcal{E}_{n,2}(t) \chi'(1)| \leq C h^{r'} \|u(t, \cdot)\|_{r+1} |\chi'(1)|\]

for $\chi \in \mathcal{S}_h$ and $t \in [0, T]$. Then, set $\chi = \theta_h$ in (4.47) and use the Cauchy-Schwarz inequality, (2.1), (4.48), (4.49), (4.43), and (2.3), to get

\[\frac{1}{2} \frac{d}{dt} \|	heta_h(t, \cdot)\|_1^2 \leq -a_1 \|	heta_h(t, \cdot)\|_1^2 + C \left[ \|	heta_h(t, \cdot)\|_1^2 + \varepsilon^{2r} \right] \Gamma_\theta(t) + \|	heta_h(t, \cdot)\|_1 \|\theta_h(t, \cdot)\|_1 \]

which, along the arithmetic-geometric mean inequality, yields

\[(4.50) \quad \frac{d}{dt} \|	heta_h(t, \cdot)\|_1^2 \leq C \left[ \|	heta_h(t, \cdot)\|_1^2 + \varepsilon^{2r} \right] \Gamma_\theta(t) \quad \forall t \in [0, T].\]

Since $\theta_h(0, \cdot) = 0$, using Grönwall’s lemma from (4.50) we see that

\[(4.51) \quad \|	heta_h(t, \cdot)\|_1^2 \leq C \varepsilon^{2r} \left( \int_0^t \Gamma_\theta(\tau) \, d\tau \right) \quad \forall t \in [0, T].\]

Finally, we combine (2.1), (4.51) and (4.37) to arrive at the error estimate (4.46). \[\square\]

### 4.2.3. Crank-Nicolson fully discrete approximations.

For $n = 0, \ldots, N$, the Crank-Nicolson method for the problem (4.1) yields an approximation $U^n_h \in \mathcal{S}_h$ of $u(t^n, \cdot)$ as follows:

**Step 1:** Set

\[(4.52) \quad U_0^n := R_h^1 u_0.\]

**Step 2:** For $n = 1, \ldots, N$, find $U^n_h \in \mathcal{S}_h$ such that

\[(4.53) \quad B(\partial U^n_h, \chi) = \left\{ \frac{a^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} (AU^n_h)'(1) - \left[ \frac{a^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} + \beta^n - \frac{1}{2} \right] (AU^n_h)(1) - \left[ \frac{a^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} + f^n - \frac{1}{2} \right] (1) \right\} \chi'(1)
\]

\[\quad + f^n - \frac{1}{2} (0) \chi'(0) - \frac{\delta^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} \beta^n - \frac{1}{2} \chi(1) + B(\beta^n - \frac{1}{2} AU^n_h, \chi) + B(\chi, B^n - \frac{1}{2}, \chi) \quad \forall \chi \in \mathcal{S}_h.\]

**Proposition 4.13.** Let $n \in \{1, \ldots, N\}$ and suppose that $U^{n-1}_h \in \mathcal{S}_h$ is well defined. If $\varepsilon^n - \frac{1}{2} > 0$, then, there exists a constant $C_n$ such that if $k_n < C_n$, then $U^n_h$ is well defined by (4.53).

**Proof.** It is enough to show that if there is a $V \in \mathcal{S}_h$ such that

\[(4.54) \quad \frac{1}{2} B(V, \phi) = \frac{1}{2} \left\{ \frac{a^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} V'(1) - \left[ \frac{a^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} + \beta^n - \frac{1}{2} \right] V(1) \right\} \phi'(1) - \frac{\delta^n - \frac{1}{2}}{\varepsilon^n - \frac{1}{2}} B^*(V, \phi) + \frac{1}{2} B(\beta^n - \frac{1}{2} V, \phi)\]
for all $\phi \in S_h$, then $V = 0$. To arrive at the desired conclusion, first set $\phi = V$ in (4.54) and use (2.1) to obtain

$$|V|^2 \leq \frac{h^2}{2} \left[ \left( 1 + \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} \right) |V'|^2 + \left( \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} + \beta^{-\frac{1}{2}}(1) \right)^2 |V(1)|^2 - a_n^{-\frac{1}{2}} |V|^2 + |\beta^{-\frac{1}{2}}|_{1, \infty} (1 + C_{\text{cf}}) |V|^2 \right].$$

Then, use (2.3), (2.4) and (4.47), to get $|V|^2 \left( 1 - \frac{2a_n}{\varepsilon - \frac{1}{2}} c_n \right) \leq 0$, where $c_n := |\beta^{-\frac{1}{2}}|_{1, \infty} (1 + C_{\text{cf}}) + 2 \left( \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} + \beta^{-\frac{1}{2}}(1) \right)^2 C_{\text{cf}} + 1 + \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} \left( 1 + \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} \right)^2$. Thus, assuming that $k_n < \frac{2}{2 + c_n}$, we easily conclude that $V = 0$. □

**Theorem 4.14.** Let $u$ be the solution of (4.1) and $(U^n_h)_{n=0}^N$ be the fully discrete approximations that the method (4.52)-(4.53) produces. If $\varepsilon(t) > 0$ for $t \in [0, T]$, then, there exists a constant $C_n \geq 0$ such that: if $\max_{1 \leq n \leq N} (k_n C_n) \leq \frac{1}{3}$, there exists a constant $C > 0$ such that

$$\max_{1 \leq n \leq N} \|U^n_h - u^n\|_1 \leq C \left( k^2 + h^r \right) \left[ \|u\|_r + \max_{|t| \leq T} \|u_{t+r}\|_1 + \max_{|t| \leq T} \|\partial_t^2 u_{t+r}\|_1 \right].$$

where

$$\gamma_{h}(u) := \min_{\ell = 0}^1 \left[ \max_{0 < t < T} \|\partial_t^\ell u\|_{r+1} + \sum_{\ell = 2}^3 \max_{\ell = 0}^{\ell} \|\partial_t^\ell u\|_{r+1} + \sum_{\ell = 4}^\infty \max_{|t| \leq T} \|\partial_t^\ell u_{t+r}\|_1 \right] \gamma(1)$$

Proof. Let $h \in (0, h_*), \theta^n_h := U^n_h - R^n_h u^n$ and $\eta^n := R^n_h u^n - u^n$ for $n = 0, \ldots, N$. Use (4.53), (4.17) and (4.35), to obtain

$$\begin{aligned}
B(\partial^\theta_h^n, \chi) &= \left\{ \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} (A(\partial_t \theta^n_h))_1 - \left( \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} + \beta^{-\frac{1}{2}}(1) \right) (A\theta^n_h)_1 + E_3 + E_4 \right\} \chi(1) \\
&\leq a_n^{-\frac{1}{2}} B^*_{\partial t} (A\theta^n_h, \chi) + B(\beta^{-\frac{1}{2}} A\theta^n_h, \chi) \\
&+ B(E^n_1 - \sigma^n, \chi) + a_n^{-\frac{1}{2}} B^* (E^n_2, \chi) + a_n^{-\frac{1}{2}} B(A\eta^n, \chi) \quad \forall \chi \in S_h, \ n = 1, \ldots, N,
\end{aligned}$$

where $\sigma^n : \mathbb{D} \rightarrow \mathbb{R}$ is defined by (4.17) and for $n = 1, \ldots, N$

$$
E^n_1 := \partial_t u^n - R^n_h \left( \partial u^n \right) - \beta^{-\frac{1}{2}} A(u^n - R^n_h u^n),
$$

$$
E^n_2 := u(t^n - \frac{1}{2}) - A u^n,
$$

$$
E^n_3 := \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} A(\partial_t \eta^n(1)) - \left( \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} + \beta^{-\frac{1}{2}}(1) \right) A(\eta^n(1)),
$$

$$
E^n_4 := \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} \left[ A(u_{t^n}(1)) - u_{t^n}(t^n - \frac{1}{2}) \right] - \left( \frac{a_n - \frac{1}{2}}{\varepsilon - \frac{1}{2}} + \beta^{-\frac{1}{2}}(1) \right) \left[ A(u(t^n, 1)) - u(t^n - \frac{1}{2}, 1) \right].
$$

Using Taylor’s formula, (4.37) and (4.38), we derive the following bounds:

$$(4.57) \quad |B(E^n_1 - \sigma^n, \chi) + a_n^{-\frac{1}{2}} B(A\eta^n, \chi)| \leq C \left[ |\sigma^n|_1 + h^r \left( \max_{|t| \leq T} \|u\|_{r+1} + \max_{|t| \leq T} \|\partial_t u\|_{r+1} \right) \right] |\chi|_1,$$

$$(4.58) \quad |\sigma^n|_1 \leq C \left( h_r \right)^2 \left( \max_{|t| \leq T} \|\partial_t^2 u\|_{r+1} + \max_{|t| \leq T} \|\partial_t^2 u\|_{r+1} \right),$$

$$(4.59) \quad |a_n^{-\frac{1}{2}} B^* (E^n_2, \chi)| \leq C h_r^r \max_{|t| \leq T} \|u\|_{r+1} \|\chi\|_1,$$

$$(4.60) \quad |E^n_3 \chi(1)| \leq C h^r + \frac{1}{2} \max_{|t| \leq T} \|u\|_{r+1} \|\chi\|_1,$$

and

$$(4.61) \quad |E^n_4 \chi(1)| \leq C h^r \left( \max_{|t| \leq T} \|\partial_t^2 u(t, 1)\| + \max_{|t| \leq T} \|\partial_t^2 \partial_t u(t, 1)\| \right) \|\chi\|_1$$

for $n = 1, \ldots, N$ and $\chi \in S_h$. 

29
Now, set $\chi = A\theta_h^n$ in (4.56) and use (2.1), the Cauchy-Schwarz inequality and the estimates (4.57), (4.59), (4.60) and (4.61), to obtain
\begin{equation}
\frac{1}{N} \left( |\theta_h^n|_1^2 - |\theta_h^{n-1}|_1^2 \right) \leq -a_s |A\theta_h^n|_1^2 + C \left[ |A\theta_h^n|_1^2 + k^2 \max_{[\theta, \tau]} \theta^2 \sigma^2 |A\theta_h^n|_2^2 \right. \\
\left. + (k^2 + h^r) \left( \mathcal{T}_n(u) \right)^2 \right. \\
\left. + |\partial_x (A\theta_h^n)(1)|^2 + |(A\theta_h^n)(1)|^2 \right], \quad n = 1, \ldots, N.
\end{equation}
(4.62)

After use of the trace inequalities (2.3) and (4.43), of the inequality (2.1) and of the arithmetic-geometric mean inequality, (4.62) yields the existence of a constant $C_n > 0$ such that
\begin{equation}
(1 - C_n k_n) |\theta_h^n|_1^2 \leq (1 + C_n k_n) |\theta_h^{n-1}|_1^2 + C k_n (k^2 + h^r)^2 \left( \mathcal{T}_n(u) \right)^2, \quad n = 1, \ldots, N.
\end{equation}
(4.63)

Assuming that $\max_{1 \leq n \leq N} (C_n k_n) \leq \frac{1}{3}$, and following a discrete Grönwall argument similar to that of Proposition 2.9, we arrive at
\begin{equation}
\max_{0 \leq n \leq N} |\theta_h^n|_1 \leq C (k^2 + h^r) \mathcal{T}_n(u).
\end{equation}
(4.64)

Thus the desired estimate (4.54) follows easily if we combine (4.64), (4.37) and (2.1). □

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References

[1] L. Abrahamsson and H. O. Kreiss, The initial boundary value problem for the Schrödinger equation, Math. Methods Appl. Sci., 13 (1990), pp. 385–390.
[2] L. Abrahamsson and H. O. Kreiss, Boundary conditions for the parabolic equation in a range-dependent duct, J. Acoust. Soc. Amer., 87 (1990), pp. 2438–2441.
[3] G. D. Akrivis and V. A. Dougalis, On a class of conservative, highly accurate Galerkin methods for the Schrödinger equation, RAIRO Model. Math. Anal. Numer., 25 (1991), pp. 643–670.
[4] G. D. Akrivis, V. A. Dougalis and G. E. Zouraris, Finite difference schemes for the ‘Parabolic’ Equation in a variable depth environment with a rigid bottom boundary condition, SIAM J. Numer. Anal., 39 (2001), pp. 539–565.
[5] D. C. Antonopoulos, Theory and numerical analysis of parabolic approximations, Ph.D. thesis, University of Athens, 2006 (in Greek).
[6] A. Bamberger, B. Engquist, L. Halpern and P. Joly, Parabolic wave equation approximations in heterogeneous media, SIAM J. Appl. Math., 48 (1988), pp. 99–128.
[7] C. Bandle, J. von Below, and W. Reichel, Parabolic problems with dynamical boundary condition: eigenvalue expansions and blow-up, Rend. Lincei Mat. Appl., 17 (2006), pp. 35–67.
[8] C. Bandle, and W. Reichel, A linear parabolic problem with non-dissipative dynamical boundary conditions, in Recent Advances on Elliptic and Parabolic Issues, Proceedings of the 2004 Swiss-Japanese Seminar, M. Chipot and H. Ninomiya eds., World Scientific, 2006, pp. 46–79.
[9] J. H. Bramble and S. R. Hilbert, Estimation of linear functionals on Sobolev spaces with application to Fourier transforms and spline interpolation, SIAM J. Numer. Anal., 7 (1970), pp. 112–124.
[10] S. C. Brenner and L. R. Scott, The Mathematical Theory of Finite Element Methods, Springer-Verlag, New York, 1994.
[11] J. Crank, The Mathematics of Diffusion, 2nd ed., Clarendon Press, Oxford, 1975.
[12] V. A. Dougalis, N. A. Kopoulos, F. Sturm, and G. E. Zouraris, Numerical solution of the Parabolic Equation in range-dependent waveguides, in Effective Computational Methods for Wave Propagation, N.A. Kampanis et al. eds., Chapman and Hall/CRC, Boca Raton, 2008, pp. 175–207.
[13] V. A. Dougalis and G. E. Zouraris, Finite difference methods for the Parabolic Equation with interface conditions, (in preparation).
[14] J. Escher, Quasilinear parabolic systems with dynamical boundary conditions, Commun. PDEs, 18 (1993), pp. 1309–1364.
[15] F. B. Jensen and C. M. Ferla, Numerical solutions of range-dependent benchmark problems in underwater acoustics, J. Acoust. Soc. Amer., 87 (1990), pp. 1499–1510.
[16] D. Lee and G. Botseas, IFD: An implicit finite-difference computer model for solving the parabolic equation, NUSC Report No. 6659, Naval Underwater Systems Center, New London, 1982.
[17] D. Lee, G. Botseas, and J. S. Papaekakis, Finite-difference solution to the parabolic wave equation, J. Acoust. Soc. Amer., 70 (1981), pp. 795–800.
[18] D. Lee and S. T. McDaniel, Ocean acoustic propagation by finite difference methods, Comput. Math. Appl., 14 (1987), pp. 305–423.
[19] J. L. Lions and E. Magenes, *Problèmes aux Limites Non Homogènes et Applications*, vol. 2, Dunod, Paris, 1968.
[20] M. B. Porter, F. B. Jensen and C. M. Ferla, *The problem of energy conservation in one-way models*, J. Acoust. Soc. Amer., 89 (1991), pp. 1058–1067.
[21] F. Sturm, *Modélisation mathématique et numérique d’un problème de propagation en acoustique sous-marine: prise en compte d’un environnement variable tridimensionnel*, Thèse de Docteur en Sciences, Université de Toulon et du Var, France, 1997.
[22] F. D. Tappert, *The parabolic approximation method*, in *Wave Propagation and Underwater Acoustics*, J.B. Keller and J.S. Papadakis, eds., Lecture Notes in Physics 70, Springer-Verlag, Berlin, 1977, pp. 224-287.
[23] V. Thomée, *Galerkin finite element methods for parabolic problems*, Springer-Verlag, Berlin, 1997.
[24] J.-L. Vázquez and E. Vitillaro, *Heat equation with dynamical boundary conditions of reactive type*, Commun. in PDEs, 33 (2008), pp. 561–612.
[25] M.-F. Wheeler, *L∞ estimates of optimal orders for Galerkin methods for one-dimensional second order parabolic and hyperbolic equations*, SIAM J. Numer. Anal., 10 (1973), pp. 908–913.