THE SHAPE DERIVATIVE FOR AN OPTIMIZATION PROBLEM IN LITHOTRIPSY

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Abstract. In this paper we consider a shape optimization problem motivated by the use of high intensity focused ultrasound in lithotripsy. This leads to the problem of designing a Neumann boundary part in the context of the Westervelt equation, which is a common model in nonlinear acoustics. Based on regularity results for solutions of this equation and its linearization, we rigorously compute the shape derivative for this problem, relying on the variational framework from [9].

1. Introduction. High intensity focused ultrasound (HIFU) has numerous applications ranging from industrial (ultrasound cleaning, welding, sonochemistry) to medical (thermotherapy, lithotripsy) ones. We will here concentrate on the latter, where high amplitude focused pressure waves are used to destroy kidney stones. The aim of achieving high pressure at the location of the stone, while keeping the pressure low in the surrounding tissue to avoid lesions, naturally leads to mathematical optimization problems, with some nonlinear acoustic wave equation for modeling HIFU as a constraint.

One of the most commonly used models in nonlinear acoustics is the Westervelt equation

\[(1 - ku)'' - c^2 \Delta u - b \Delta u' = 0\] (1)

where \(u\) is the acoustic pressure, \(c > 0\) the speed of sound, \(b > 0\) the diffusivity of sound, \(\varrho > 0\) the mass density, and \(k > 0\) a parameter quantifying the nonlinearity. Here and below a prime \(\prime\) denotes the derivative with respect to time.

The two most widely used excitation and focusing principles are based on either:

a) excitation by a magnetomechanical principle and focusing by an acoustic lens, see Figure 1, left.

b) excitation by an array of piezoelectric transducers arranged in a spherical calotte and aimed at the focus point (self-focusing), see Figure 1, right.

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Here we shall concentrate on the latter principle (b), whereas the former one (a), requiring modeling by a coupled system of PDEs for the lens and the surrounding fluid, is investigated in [10].

Excitation by the piezoelectric transducers is modeled by the Neumann boundary conditions
\[
\frac{\partial u}{\partial \nu} = g \quad \text{on } (0, T) \times \Gamma_n,
\]
where \(\Gamma_n\) represents the surface composed by the piezoelectric transducers. In order to be able to restrict the open domain problem of (nonlinear) acoustics to a smooth and bounded domain \(\Omega \subseteq \mathbb{R}^3\) (which has obvious computational advantages), we employ first order absorbing boundary conditions on the rest of the boundary \(\Gamma_a = \partial \Omega \setminus \Gamma_n\)
\[
\frac{1}{c} u' + \frac{\partial u}{\partial \nu} = 0 \quad \text{on } (0, T) \times \Gamma_a
\]
For higher order absorbing boundary conditions for the Westervelt equation we refer to [11]. The boundary optimal control problem dealing with an optimal choice of the excitation pattern \(g\) in (2) has been considered in [5] and [4]. Here we will, for a given prescribed \(g\), consider the problem of finding an optimal shape of the piezoarray, i.e., of \(\Gamma_n\), which is of practical relevance due to the fact that the range of achievable excitation patterns \(g\) is limited in some devices.

As in [5] and [10] the goal of the optimization is to achieve a prescribed pressure distribution \(y_d\), i.e., considering the domain \(\Omega\) as a design variable, we seek to minimize the cost functional
\[
J(u, \Omega) = \int_0^T \int_{\Omega} (u - y_d)^2 \, dx \, d\sigma = \int_0^T \int_{\Omega} j(u) \, dx \, d\sigma,
\]
with the PDE model (1), (2), (3) as a constraint.

The remainder of the paper is organized as follows. Section 2 contains some results on the nonlinear PDE as well as its linearization, that will be made use of later on. In Section 3 we will provide the framework for domain variation and some useful tools for this purpose. Our main result is contained in Section 4, where we carry out a shape sensitivity analysis for the optimization problem described above.

**Figure 1.** Excitation and focusing principles
and provide an expression for the Eulerian derivative of the cost functional (4) with respect to variations of the domain.

**Notation.** Below we shall frequently use the short hand notation $X(Y)$ for spaces of vector valued functions $X(0,T;Y(\Omega))$ and we will abbreviate the $L^2$ inner product on $\Omega$ by $(\cdot,\cdot)$. The embedding constant of $H^1(\Omega)$ into $L^p(\Omega)$ will be denoted by $C_{\Omega,p}$, $1 \leq p \leq 6$, the one of $H^{1/2}(\Gamma_n)$ into $L^p(\Omega)$ by $C_{\Gamma_n,p}$, $1 \leq p \leq 4$, the norm of the trace operators $tr_{\Gamma_n} : H^1(\Omega) \to H^{1/2}(\Gamma_n)$, $tr_{\Gamma_n} : H^1(\Omega) \to H^{1/2}(\Gamma_n)$ by $C_{\text{tr},\Gamma_n}$, $C_{\text{tr},\Gamma_n}$.

### 2. Some properties of the PDE model.

In this section we consider the Westervelt equation on a fixed bounded $C^{1,1}$-domain $\Omega \subset \mathbb{R}^3$ with boundary conditions (2), (3)

$$
((1 - ku)u')' - c^2 \Delta u - b\Delta u' = 0 \quad \text{in } (0,T) \times \Omega,
$$

$$
\frac{1}{c} u' + \frac{\partial u}{\partial \nu} = 0 \quad \text{on } (0,T) \times \Gamma_a,
$$

$$
\frac{\partial u}{\partial \nu} = g \quad \text{on } (0,T) \times \Gamma_n,
$$

$$
u(0) = u_0, \quad u_1(0) = u_1 \quad \text{in } \Omega
$$

under the following assumptions

1. $u_0 \in H^2(\Omega)$, $u_1 \in H^1(\Omega)$
2. $c^2g + bg' \in H^1(0,T;H^{-1/2}(\Gamma_n))$, $g \in L^\infty(0,T;H_0^1(\Gamma_n))$ for some $s \in (0,\frac{1}{2})$

(H3) compatibility conditions

- $\frac{1}{c} u_1 + \frac{\partial u}{\partial \nu} = 0$ on $\Gamma_a$,
- $\frac{\partial u}{\partial \nu} = g(0)$ on $\Gamma_n$.

(H4) $\partial \Gamma_n$ and $\partial \Gamma_n$ are Lipschitz.

For a given function $y$ we associate with (5) the following linear initial boundary value problem

$$
((1 - 2ky)\xi')' - c^2 \Delta \xi - b\Delta \xi' = f \quad \text{in } (0,T) \times \Omega,
$$

$$
\frac{1}{c} \xi' + \frac{\partial \xi}{\partial \nu} = 0 \quad \text{on } (0,T) \times \Gamma_a,
$$

$$
\frac{\partial \xi}{\partial \nu} = g \quad \text{on } (0,T) \times \Gamma_n.
$$

\xi(0) = \xi_0, \quad \xi_1(0) = \xi_1,

which can be regarded as a linearization of (5) with an additional inhomogeneity $f$.

Well-posedness of (5) and (6) has already been stated in [5]. However, the argument leading from $L^2$ regularity of $\Delta u$ to $H^{3/2+s}$ regularity of $u$ (which together with the embedding $H^{3/2+s}(\Omega) \to L^\infty(\Omega)$ is crucial for avoiding degeneracy of the coefficient $(1 - 2ku)$ of the second time derivative) had been missing in [5].

**Theorem 1.** Let $T \in (0,\infty)$ and let the following conditions on the data

- $\xi_0, \xi_1 \in H^1(\Omega)$,
- $c^2g + bg' \in H^1(0,T;H^{-1/2}(\Gamma_n))$
- $f \in H^1(0,T;H^1(\Omega)^*)$
- $y \in C^1([0,T],L^2(\Omega)) \cap W^{1,\infty}(0,T;L^3(\Omega)) \cap C([0,T],L^\infty(\Omega))$

hold and assume that $y$ is small in the sense that

- $\|y\|_{L^\infty(0,T;L^\infty(\Omega))} \leq \frac{1}{16}$
Then the initial boundary value problem (6) has a unique weak solution

\[ \xi \in X := \{ \phi \in H^2(0, T; L^2(\Omega)) \cap W^{1,\infty}(0, T; H^1(\Omega)) : (\iota_{\Gamma_a} \phi')' \in L^2(0, T; L^2(\Gamma_a))\} \]

and \(\xi\) satisfies the energy estimates

\[
\|\xi'(s)\|_{L^2(\Omega)}^2 + \|\nabla \xi(s)\|_{L^2(\Omega)}^2 + \|\iota_{\Gamma_a} \xi'(s)\|_{L^2(\Gamma_a)}^2 + \int_0^s \|\xi''(s)\|_{H^1(\Omega)}^2 \, ds \leq C_1(\|\xi_0\|_{H^1(\Omega)})^2 + \|\xi_1\|_{H^1(\Omega)}^2 + \|c^2 g + b g'\|_{L^2(0, T; H^{-1/2}(\Gamma_n))}^2 + \|f\|_{L^2(0, T; (H^1(\Omega)'))}^2.
\]

\[
\|\nabla \xi(s)\|_{L^2(\Omega)}^2 + \int_0^s \|\xi'(s)\|_{H^1(\Omega)}^2 \, ds + \|\xi'(s)\|_{H^1(\Omega)}^2 \, ds \leq C_2(1 + \|\xi'(s)\|_{L^2(0, T; L^2)}^2)(\|\xi_0\|_{H^1(\Omega)})^2 + \|\xi_1\|_{H^1(\Omega)}^2 + \|c^2 g + b g'\|_{L^\infty(0, T; H^{-1/2}(\Gamma_n))}^2 + \|f\|_{L^\infty(0, T; (H^1(\Omega)'))}^2.
\]

with constants \(C_1, C_2\) independent of \(T\).

If additionally for some \(s \in (0, \frac{T}{2})\)

- \(\xi_0 \in H^2(\Omega),\)
- \(g \in L^\infty(0, T; H^0_0(\Gamma_n))\)
- \(f \in L^1(0, T; L^2(\Omega))\)

and the compatibility conditions

\[
\frac{1}{c} \xi_1 + \frac{\partial \xi_0}{\partial \nu} = 0, \quad \quad (10)
\]

\[
\frac{\partial \xi_0}{\partial \nu} = g(0), \quad \text{on } \Gamma_n, \quad \quad (11)
\]

as well as \((H_4)\) are satisfied, then we have

\[ \xi \in L^\infty(0, T; H^{3/2+s}(\Omega)) \subseteq L^\infty(0, T; C(\Omega)). \]

Proof. The proof is divided into five steps. We start with a Galerkin approximation of the weak form of the PDE by restriction to appropriate finite dimensional subspaces of \(H^1(\Omega)\), i.e., we do a semidiscretization with respect to space and establish well-posedness of the resulting system of ODEs. For these solutions, we derive energy estimates of first (Step 2) and second (Step 3) order with respect to time. These estimates enable to extract a weakly convergent subsequence in appropriate spaces, whose limit we prove to solve the weak form of the PDE in Step 4. Finally, we prove higher order regularity in space, which is crucial for avoiding degeneracy in the nonlinear equation later on.

For convenience we shall use the notation

\[ a = 1 - 2ky. \]
for which by assumption \(i\)

\[
\frac{1}{2} \leq a(\sigma) \leq \frac{3}{2} \quad \text{a.e. in } \Omega \tag{12}
\]

holds for all \(\sigma \in [0, T]\). Then the weak form of (6) is given by

\[
((a\xi', v) + (c^2 \nabla \xi + b \nabla \xi', \nabla v) + \int_{\Gamma_n} (c\xi' + \frac{b}{c} \xi'') v \, d\gamma = \int_{\Gamma_n} (c^2 g + bg') v \, d\gamma + (f, v), \quad v \in H^1(\Omega), \quad \text{for a.e. } \sigma \in (0, T)
\]

\[
\xi(0) = \xi_0, \quad \xi'(0) = \xi_1 \quad \text{in } \Omega
\]  

We mention that the term \(\int_{\Gamma_n} \xi'' v \, d\gamma\) should be interpreted as \(\int_{\Gamma_n} (\text{tr}_{\Gamma_n} \xi')' v \, d\gamma\) where \(\text{tr}_{\Gamma_n}\) is the trace operator on \(\Gamma_n\).

**Step 1. Galerkin approximation.** Following the Faedo-Galerkin technique (see, e.g. [7]) we choose a complete sequence of linearly independent elements \(w_i \in H^1(\Omega), i \in \mathbb{N}\). Let \(V_n\) denote the span of \(\{w_1, \ldots, w_n\}\) and define

\[
\xi_n(\sigma) = \sum_{k=1}^{n} \alpha_k^n(\sigma) w_k, \quad \xi_n(0) = \xi_0^n, \quad \xi_n'(0) = w_1^n
\]

where \(\xi_0^n, \xi_1^n \in V_n\) converge to \(\xi_0, \xi_1\) in \(H^1(\Omega)\). The coefficients \(\alpha_k^n\) are determined by the approximate equation

\[
((a\xi_n', w_i) + (c^2 \nabla \xi_n + b \nabla \xi_n', \nabla w_i) + \int_{\Gamma_n} (c\xi_n' + \frac{b}{c} \xi_n'') w_i \, d\gamma = \int_{\Gamma_n} (c^2 g + bg') w_i \, d\gamma + (f, w_i), \quad i \in \mathbb{N}, \quad \sigma \in (0, T)
\]

\[
\xi_n(0) = \xi_0^n, \quad \xi_n'(0) = \xi_1^n
\]

which is equivalent to

\[
\sum_{k=1}^{n} ((a_k^n)'(aw_k, w_i) + (a_k^n)'(a'w_k, w_i) + c^2 a_k^n(\nabla w_k, \nabla w_i) + b(\alpha_k^n)'(\nabla w_k, \nabla w_i) + (c(\alpha_k^n)' + \frac{b}{c} (\alpha_k^n)') \int w_k w_i = \int_{\Gamma_n} (c^2 g + bg') w_i \, d\gamma + (f, w_i).
\]

\[
\alpha_k^n(0) = \beta_k^n, \quad \alpha_k^n'(0) = \gamma_k^n
\]

Above \(\beta_k^n, \gamma_k^n\) denote the components of \(\xi_0^n\), respectively \(\xi_1^n\) with regard to \(\{w_1, \ldots, w_n\}\). Define \(A, B : [0, T] \rightarrow \mathbb{R}^{n \times n}, M, N \in \mathbb{R}^{n \times n}, F^\alpha : [0, T] \rightarrow \mathbb{R}^n\) by

\[
A_{ki}(\sigma) = (a(\sigma) w_k, w_i), \quad B_{ki}(\sigma) = (a'(\sigma) w_k, w_i)
\]

\[
M_{ki} = \langle \nabla w_k, \nabla w_i \rangle, \quad N_{ki} = \int_{\Gamma_n} w_k w_i
\]

\[
\alpha^n(\sigma) = (\alpha^n_1(\sigma), \ldots, \alpha^n_n(\sigma)), \quad F^\alpha_k(\sigma) = \int_{\Gamma_n} (c^2 g + bg') w_k \, d\gamma + (f(\sigma), w_k).
\]

We note that all these quantities and in particular \(A_{kj}(\sigma)\) and \(B_{kj}(\sigma)\) are well defined. This is a consequence of \(a \in C^1([0, T], L^2(\Omega))\) and the embedding of \(H^1(\Omega)\)
into $L^4(\Omega)$ (with embedding constant $C_{1,4} > 0$) which, by the generalized Hölder inequality, implies

$$|(a(\sigma)w_k, w_i)| \leq |a(\sigma)|_{L^2(\Omega)} |w_k|_{L^4} |w_i|_{L^4} \leq C_{1,4}^2 |a(\sigma)|_{L^2(\Omega)} \|w_k\|_{H^1(\Omega)} \|w_i\|_{H^1(\Omega)}$$

and similarly for $|(a'(\sigma)w_k, w_i)|$ for every $\sigma \in [0, T]$. For simplicity we shall write $\alpha, \beta, \gamma, F$ instead of $\alpha^n, \beta^n, \gamma^n, F^n$.

We note that $A$ is positive definite for every $\sigma \in [0, T]$: For any $\sigma \in [0, T]$, $y \in \mathbb{R}^n \setminus \{0\}$ and $u = \sum_{i=1}^n y_i w_i$ we find

$$y^T A(\sigma) y = \int_\Omega a u^2 \geq \frac{1}{2} |u|_{L^2(\Omega)}^2 > 0,$$

by (12) and the linear independence of $\{w_1, \ldots, w_n\}$.

Thus $\alpha$ satisfies the following system of ordinary differential equations

$$(A(\sigma) + \frac{b}{c} N)\alpha'' + (B(\sigma) + bM + cN)\alpha' + c^2 M \alpha = F,$$

$$\alpha(0) = \beta, \quad \alpha'(0) = \gamma.$$ 

Since $N$ is nonnegative, the matrix $A(\sigma) + \frac{b}{c} N$ is invertible for every $\sigma \in [0, T]$ and the above system is equivalent to

$$\alpha'' + (A(\sigma) + \frac{b}{c} N)^{-1} (B(\sigma) + bM + cN)\alpha' + c^2 (A(\sigma) + \frac{b}{c} N)^{-1} M \alpha = (A(\sigma) + \frac{b}{c} N)^{-1} F(\sigma)$$

$$\alpha(0) = \beta, \quad \alpha'(0) = \gamma.$$ 

This equation has a unique solution $\alpha \in H^2((0, T), \mathbb{R}^n)$. Since the coefficients of the equation and the right hand side at least belong to $C((0, T), \mathbb{R}^n)$ we even find $\alpha \in C^2((0, T), \mathbb{R}^n)$. Hence we obtain that the equation

$$((a\xi_n', v) + (c^2 \nabla \xi_n + b \nabla \xi_n', \nabla v) + \int_{\Gamma_n} (c\xi_n' + \frac{b}{c} \xi_n'')v$$

$$= \int_{\Gamma_n} (c^2 g + bg')v \, d\gamma + (f, v), \quad v \in V_n$$

$$\xi_n(0) = \xi_0^n, \quad \xi_n'(0) = \xi_1^n$$

has a unique solution $\xi_n \in C^2(H^1)$

**Step 2. lower order energy estimate.** We insert $w = \alpha_i' w_i$ into (17), take the sum over $i$ and integrate from zero to $s$ to obtain

$$\int_0^s \left[ ((a\xi_n', \xi_n') + c^2 (\nabla \xi_n, \nabla \xi_n') + b|\nabla \xi_n|^2_{L^2(\Omega)} + \int_{\Gamma_n} (c\xi_n' + \frac{b}{c} \xi_n'')\xi_n' \right] \, d\sigma$$

$$= \int_0^s \left[ \int_{\Gamma_n} (c^2 g + bg')\xi_n' \, d\gamma + (f, \xi_n') \right] \, d\sigma.$$ 

In view of the identity

$$(a\xi_n')\xi_n' = a\xi_n''\xi_n + \frac{1}{2}(a\xi_n')^2 = \frac{1}{2}(a\xi_n')^2 + \frac{1}{2}a'(\xi_n')^2$$
one finds
\[ \int_{0}^{s} \left[ \frac{1}{2} \frac{d}{d\sigma} (a' \xi'_n, \xi'_n) + \frac{1}{2} (a' \xi'_n, \xi'_n) + \frac{c^2}{2} \frac{d}{d\sigma} \| \nabla \xi_n(\sigma) \|_{L^2(\Omega)}^2 + b \| \nabla \xi'_n \|_{L^2(\Gamma_n)}^2 \right] \, d\sigma + c \| \xi'_n \|_{L^2(\Gamma_n)}^2 \, d\sigma + \frac{b}{2c} \| \xi'_n \|_{L^2(\Gamma_n)}^2 \right] \, d\sigma \]
\[ = \int_{0}^{s} \left[ \int_{\Gamma_n} (c^2 g + bg') \xi'_n \, d\gamma + (f, \xi'_n) \right] \, d\sigma. \]
which is equivalent to
\[ \frac{1}{2} \sqrt{a(s)} \xi'_n(\sigma) \|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{0}^{s} (a' \xi'_n, \xi'_n) \, d\sigma + \frac{c^2}{2} \| \nabla \xi_n(\sigma) \|_{L^2(\Omega)}^2 \]
\[ + b \int_{0}^{s} \| \nabla \xi'_n \|_{L^2(\Omega)}^2 \, d\sigma + c \int_{0}^{s} \| \xi'_n \|_{L^2(\Gamma_n)}^2 \, d\sigma + \frac{b}{2c} \| \xi'_n \|_{L^2(\Gamma_n)}^2 \]
\[ = \frac{1}{2} \sqrt{a(0)} \xi'_n(\sigma) \|_{L^2(\Omega)}^2 + \frac{c^2}{2} \| \nabla \xi'_n \|_{L^2(\Omega)}^2 + \frac{b}{2c} \| \xi'_n \|_{L^2(\Gamma_n)}^2 \]
\[ + \int_{0}^{s} \left[ \int_{\Gamma_n} (c^2 g + bg') \xi'_n \, d\gamma + (f, \xi'_n) \right] \, d\sigma. \]
which holds for all \( s \in [0, T] \). From (15) we infer
\[ \| (a' \xi'_n, \xi'_n) \|_{L^2(\Omega)} \leq C_1 \| \xi'_n \|_{L^2(\Omega)} \leq C_2 \| \xi'_n \|_{H^1(\Omega)}. \]

Since \( \xi_n^0, \xi_n^1 \) converge to \( \xi_0, \xi_1 \) in \( H^1(\Omega) \) we may assume for \( n \) sufficiently large
\[ \| \xi_n^0 \|_{H^1(\Omega)} \leq \sqrt{2} \| \xi_0 \|_{H^1(\Omega)}, \quad \| \xi_n^1 \|_{H^1(\Omega)} \leq \sqrt{2} \| \xi_1 \|_{H^1(\Omega)}. \]

In view of (12) and the estimate
\[ \left| \int_{\Gamma_n} \left( \int_{\Gamma_n} (c^2 g + bg') \xi'_n \, d\gamma + (f, \xi'_n) \right) \, d\sigma \right| \]
\[ \leq \frac{1}{2c} C_{tr, \Gamma_n}^2 \| c^2 g + bg' \|_{L^2(\Omega)} \, d\sigma \]
\[ \leq \frac{1}{2c} \left( C_{tr, \Gamma_n}^2 \| \nabla \xi'_n \|_{L^2(\Omega)}^2 + \frac{b}{2c} \| \xi'_n \|_{L^2(\Gamma_n)}^2 \right) \, d\sigma. \]

as well as the fact that
\[ \| \xi'_n \|_{H^1(\Omega)} \leq \frac{1}{2c} \| \nabla \xi'_n \|_{L^2(\Omega)} \, d\sigma. \]

defines an equivalent norm on \( H^1(\Omega) \) (2, p 298 and Example 7.3.15), hence,
\[ \| \varphi \|_{H^1(\Omega)} \leq C_{eq, \Gamma_n} \| \varphi \|_{H^1(\Omega)}, \quad \varphi \in H^1(\Omega) \]

for some constant \( C_{eq, \Gamma_n} > 0 \), we obtain
\[ \frac{1}{2} \| \xi'_n \|_{L^2(\Omega)}^2 + \frac{c^2}{2} \| \nabla \xi_n(s) \|_{L^2(\Omega)}^2 + \frac{b}{2c} \| \xi'_n \|_{L^2(\Gamma_n)}^2 + \frac{\min(b, c)}{2C_{tr, \Gamma_n}} \int_{0}^{s} \| \xi'_n \|_{H^1(\Omega)}^2 \, d\sigma \]
\[ \leq c^2 \| \xi_0 \|_{H^1(\Omega)} + \frac{1}{2} \left( \frac{3}{2} + \frac{b}{c} C_{tr, \Gamma_n} \right) \| \xi_1 \|_{H^1(\Omega)} + \frac{1}{2c} \| \xi'_n \|_{H^1(\Omega)}^2 \]
\[ + \frac{1}{2c} \| f \|_{L^2(\Omega)} + \left( \frac{\min(b, c)}{2C_{tr, \Gamma_n}} \right) \| a' \|_{L^\infty(L^2)} \, d\sigma. \]

The choice \( \varepsilon = \frac{\min(b, c)}{4C_{tr, \Gamma_n}} \) and assumption ii) implies
\[ \frac{1}{2} C_{tr, \Gamma_n}^2 \| a' \|_{L^\infty(L^2)} + \varepsilon \leq \frac{\min(b, c)}{2C_{eq, \Gamma_n}}. \]
Due to (12) and the estimates

\[ \|\xi_n(s)\|_{L^2(\Omega)}^2 + \|\nabla \xi_n(s)\|_{L^2(\Omega)}^2 + \|\xi'_n(s)\|_{L^2(\Gamma_n)}^2 + \int_0^s \|\xi'_n\|_{H^1(\Omega)}^2 \, d\sigma \]

\[ \leq \kappa_c^2 \|\xi_0\|_{H^1(\Omega)}^2 + \kappa_c \left( \frac{3}{2} + \frac{b}{c} \right) \|\xi_1\|_{H^1(\Omega)}^2 \]

\[ + \kappa_c^2 C_{tr,\Gamma_n}^2 \|\xi_n\|_{H^2(\Gamma_n)}^2 \]

\[ \leq C_1(\|\xi_0\|_{H^1(\Omega)}^2 + \|\xi_1\|_{H^1(\Omega)}^2 + \|\xi_n\|_{H^2(\Gamma_n)}^2 + \|f\|_{L^2((H^1)')}^2) \]

(18)

**Step 3. Higher order energy estimate.** In order to derive estimates for the second time derivative we test (17) with \( v = \xi_n'' \), which after integration by parts with respect to time of some of the terms gives

\[ \int_0^s (a\xi_n'' + c\nabla^2 \xi_n) \, d\sigma + \frac{b}{c} \int_0^s \|\nabla \xi_n(s)\|_{L^2(\Gamma_n)}^2 \, d\sigma + \frac{c}{2} \|\xi'_n(s)\|_{L^2(\Gamma_n)}^2 \]

\[ = -c^2 (\nabla \xi_n(s), \nabla \xi_n(s)) + c^2 (\nabla \xi_n', \nabla \xi_n') + \frac{b}{2} \|\nabla \xi_n'(s)\|_{L^2(\Omega)}^2 + \frac{c}{2} \|\xi''_n(s)\|_{L^2(\Gamma_n)}^2 \]

\[ + c^2 \int_0^s \|\nabla \xi_n'(s)\|_{L^2(\Omega)}^2 \, d\sigma + \int_{\Gamma_n} (c^2 g + bg')(0) \xi_n''(s) \, d\gamma - \int_{\Gamma_n} (c^2 g + bg')(0) \xi_n'(s) \, d\gamma \]

\[ - \int_0^s \int_{\Gamma_n} (c^2 g' + bg'')(s) \xi_n'(s) \, d\gamma \, d\sigma - \int_0^s (a\xi_n', \xi_n'') \, d\sigma \]

\[ + (f(s), \xi_n'(s)) - (f(0), \xi_n') - \int_0^s (f', \xi_n') \, d\sigma \]

(19)

Due to (12) and the estimates

\[ \left| c^2 (\nabla \xi_n', \nabla \xi_n') + \frac{b}{2} \|\nabla \xi_n'\|_{L^2(\Omega)}^2 + \frac{c}{2} \|\xi'_n\|_{L^2(\Gamma_n)}^2 \right| \]

\[ \leq C_0(\|\xi_0\|_{H^1(\Omega)}^2 + \|\xi_1\|_{H^1(\Omega)}^2 + \|c^2 g + bg'(0)\|_{H^{-1/2}(\Gamma_n)}^2 + \|f(0)\|_{H^1(\Omega)}^2) \]

\[ \int_{\Gamma_n} (c^2 g + bg')(s) \xi_n'(s) \, d\gamma \leq \frac{C_{tr,\Gamma_n}}{\varepsilon_1} \|c^2 g + bg'(0)\|_{H^{-1/2}(\Gamma_n)}^2 + \varepsilon_1 \|\xi_n'(s)\|_{H^1(\Omega)}^2 \]

\[ \int_0^s \int_{\Gamma_n} (c^2 g' + bg'')(s) \xi_n'(s) \, d\gamma \, d\sigma \]

\[ \leq \frac{C_{tr,\Gamma_n}^2}{4\varepsilon_2} \|c^2 g' + bg''\|_{L^2((H^{-1/2}(\Gamma_n)))}^2 + \varepsilon_2 \int_0^s \|\xi_n'(s)\|_{H^1(\Omega)}^2 \, d\sigma \]

\[ \int_0^s (a\xi_n', \xi_n'') \, d\sigma \leq \int_0^s \|a\|_{L^\infty(\Omega)} \|\xi_n'\|_{L^\infty(\Omega)} \|\xi_n''\|_{L^2(\Omega)} \, d\sigma \]

\[ \leq \frac{C_{\Omega,6}}{4\varepsilon_3} \|a\|^2_{L^\infty(L^3)} \int_0^s \|\xi_n''\|_{H^1(\Omega)}^2 \, d\sigma + \varepsilon_3 \int_0^s \|\xi_n''\|_{L^2(\Omega)}^2 \, d\sigma \]

\[ |(f(s), \xi_n(s))| \leq \frac{1}{4\varepsilon_4} \|f(s)\|_{H^1(\Omega)}^2 + \varepsilon_4 \|\xi_n(s)\|_{H^1(\Omega)}^2 \]

\[ \int_0^s (f', \xi_n'^2) \, d\sigma \leq \frac{1}{4\varepsilon_5} \|f'\|_{L^2((H^1(\Omega)))^*}^2 + \varepsilon_5 \int_0^s \|\xi_n''\|_{H^1(\Omega)}^2 \, d\sigma \]
\( (19) \) implies

\[
\frac{1}{2} \int_0^s \| \xi''_n \|^2_{L^2(\Omega)} \, ds + \frac{b}{c} \int_0^s \| \xi'_n \|^2_{L^2(\Gamma_n)} \, ds + \frac{\min(b, c)}{2C_{\text{eq}, \Gamma_n}} \| \xi'_n(s) \|^2_{H^1(\Omega)} \\
\leq C_0(\| \xi_0 \|^2_{H^1(\Omega)} + \| \xi_1 \|^2_{H^1(\Omega)} + \| (c^2 g + bg')(0) \|^2_{H^{-1/2}(\Gamma_n)} + \| f(0) \|^2_{H^1(\Omega)}^*) \\
+ \frac{C^2_{\text{tr}, \Gamma_n}}{4\varepsilon_1} \| (c^2 g + bg')(s) \|^2_{H^{-1/2}(\Gamma_n)} + \frac{C^2_{\text{tr}, \Gamma_n}}{4\varepsilon_2} \| c^2 g' + bg'' \|^2_{L^2(\Omega)} \\
+ \frac{1}{4\varepsilon_4} \| f(s) \|^2_{H^1(\Omega)^*} + \frac{1}{4\varepsilon_5} \| f' \|^2_{L^2((H^1(\Omega))^*)} \\
+ \varepsilon_3 \int_0^s \| \xi''_n \|^2_{L^2(\Omega)} \, ds + (\varepsilon_1 + \varepsilon_4) \| \xi'_n(s) \|^2_{H^1(\Omega)} \\
+ \left( \varepsilon_2 + \frac{C^2_{\text{tr}, \Gamma_n}}{4\varepsilon_3} \| a' \|^2_{L^\infty(L^2)} + \varepsilon_5 + c^2 \right) \int_0^s \| \xi'_n \|^2_{H^1(\Omega)} \, ds.
\]

Setting \( \varepsilon_1 = \varepsilon_4 = \frac{\min(b, c)}{2C_{\text{eq}, \Gamma_n}}, \varepsilon_3 = \frac{1}{4}, \varepsilon_2 = \varepsilon_5 = 1 \) and adding \( \lambda \) times \((18)\) with \( \lambda = \frac{5}{2} + \frac{C^2_{\text{tr}, \Gamma_n}}{4\varepsilon_3} \| a' \|^2_{L^\infty(L^2)} + c^2 \), we obtain

\[
\| \nabla \xi_n(s) \|_{L^2(\Omega)} + \int_0^s \| \xi'_n \|^2_{H^1(\Omega)} \, ds + \| \xi'_n(s) \|^2_{H^1(\Omega)} \\
+ \int_0^s \| \xi''_n \|^2_{L^2(\Omega)} \, ds + \int_0^s \| \xi''_n \|^2_{L^2(\Gamma_n)} \, ds \\
\leq C_2 (1 + \| a' \|^2_{L^\infty(L^2)}) \left( \| \xi_0 \|^2_{H^1(\Omega)} + \| \xi_1 \|^2_{H^1(\Omega)} + \| c^2 g + bg' \|^2_{L^\infty(H^{-1/2}(\Gamma_n))} \\
+ \| c^2 g + bg' \|^2_{H^1(H^{-1/2}(\Gamma_n))} + \| f \|^2_{L^\infty((H^1(\Omega))^*)} + \| f \|^2_{H^1((H^1(\Omega))^*)} \right),
\]

which holds for all \( s \in [0, T] \). In particular, since

\[
\| \xi_n(s) \|_{L^2(\Omega)} = \| \xi_n(0) \|_{L^2(\Omega)} + \int_0^s \| \xi'_n(\sigma) \|_{L^2(\Omega)} \, d\sigma \leq \| \xi_0 \|_{L^2(\Omega)} + \sqrt{T} \| \xi_n''(s) \|_{L^2(\Omega)},
\]

we can bound the full \( H^1 \) norm of \( \xi_n \), so altogether \( \xi_n \) is bounded in \( H^1(L^2) \cap H^2(L^2) \) and \( (\text{tr}_{\Gamma_n} \xi'_n) \) is bounded in \( L^2(L^2(\Gamma_n)) \). Therefore there exist a subsequence, again denoted by \( \xi_n \), and \( \xi \in H^1(L^2) \cap H^2(L^2), y \in L^2(L^2(\Gamma_n)) \) such that

\[
\xi_n \rightarrow \xi \quad \text{in} \quad H^1(L^2) \cap H^2(L^2) \\
\text{tr}_{\Gamma_n} \xi_n' \rightarrow \text{tr}_{\Gamma_n} \xi' \quad \text{in} \quad L^2(H^{1/2}(\Gamma_n)) \\
\xi_n \rightarrow \xi \quad \text{in} \quad C(L^2) \\
(\text{tr}_{\Gamma_n} \xi_n')' \rightarrow y \quad \text{in} \quad L^2(L^2(\Gamma_n)).
\]

where the second line follows from the first one due to boundedness and linearity, hence weak continuity, of the trace operator \( H^1(\Omega) \rightarrow H^{1/2}(\Gamma_n) \), and the third line from compactness of the embedding of \( H^1(\Omega) \) into \( C(L^2) \). Additionally, it can be seen that the limit in the fourth line coincides with the derivative of the trace of \( \xi' \). Namely, denoting by \( (\cdot, \cdot)_{\Gamma_n} \) the inner product in \( L^2(\Gamma_n) \), we get, for any
\( v \in L^2(\Gamma_a), \phi \in C^0_0(0,T), \)
\[
\lim_{n \to \infty} \int_0^T \int_{\Gamma_a} (\text{tr}_a \xi_n') y \, d\gamma \phi \, d\sigma = \lim_{n \to \infty} \int_0^T (\text{tr}_a \xi_n) , v)_{\Gamma_a} \phi \, d\sigma = \lim_{n \to \infty} \int_0^T (\text{tr}_a \xi_n') \phi \, d\sigma = -\lim_{n \to \infty} \int_0^T \text{tr}_a \xi_n' \phi \, d\sigma = -\int_0^T \text{tr}_a \xi' \phi \, d\sigma - \int_0^T \phi \, d\sigma.
\]

The last equality is justified by the fact that \((\text{tr}_a \xi_n')\) converges weakly in \(L^2(L^2(\Gamma_a))\) to \(\text{tr}_a \xi'\). On the other hand, by the last line in (22),
\[
\lim_{n \to \infty} \int_0^T (\text{tr}_a \xi_n') , v)_{\Gamma_a} \phi \, d\sigma = \int_0^T (y, v)_{\Gamma_a} \phi \, d\sigma = (\int_0^T y \phi \, d\sigma, v)_{\Gamma_a}
\]
which, since \(v \in L^2(\Gamma_a)\) was arbitrary, implies
\[
\int_0^T \text{tr}_a \xi' \phi \, d\sigma = - \int_0^T \phi \, d\sigma, \quad \phi \in D(0,T),
\]

hence
\[
(\text{tr}_a \xi') = y \in L^2(L^2(\Gamma_a)). \quad (23)
\]

**Step 4. Weak limits and verification of PDE.** Define for arbitrary but fixed \(\phi \in C^1([0,T]), v \in H^1(\Omega)\) the functional
\[
\langle \ell_{\phi,v}^*, z \rangle = \int_0^T \left[ \left\{ (az')', v \right\} + (c^2v + b\nabla z', \nabla v) \right] \phi \, d\sigma
\]
for \(z \in H^1(\Omega) \cap H^2(L^2)\). In view of
\[
|\langle \ell_{\phi,v}^*, z \rangle| \leq \|\phi\|_{L^2(\Omega)} \|v\|_{H^1(\Omega)} (\max(c^2, b) + cC^2_{\nabla,\Gamma_a} + C^2_{\nabla,\nabla} a' \|L^\infty(L^2)\| + \|a\|_{L^\infty(L^\infty)})
\]

\[
\cdot \left( \|z\|_{H^1(\Omega)} + \|z\|_{H^2(L^2)} \right),
\]

one finds \(\ell_{\phi,v}^* \in (H^1(\Omega) \cap H^2(L^2))^*\) which by (22) implies \(\lim_{n \to \infty} \langle \ell_{\phi,v}^*, \xi_n \rangle = \langle \ell_{\phi,v}^*, \xi \rangle\), i.e.,
\[
\lim_{n \to \infty} \int_0^T \left[ \left\{ (a\xi_n')', v \right\} + (c^2v + b\nabla \xi_n', \nabla v) \right] \phi \, d\sigma = \int_0^T \left[ \left\{ (a\xi')', v \right\} + (c^2v + b\nabla \xi', \nabla v) \right] \phi \, d\sigma.
\]

Here we have used the fact that for \(a \in L^\infty(L^2) \cap H^1(L^3)\) and \(\xi' \in H^1(L^2) \cap L^2(L^6)\) the distributional product rule is applicable and yields \(a\xi'' + a'\xi' = (a\xi')'\), since with an approximating sequence \((a_k)_{k \in \mathbb{N}} \subseteq C^\infty_0([0,T];C^0_0(\Omega))\), \(a_k \to a\) in
$L^\infty(L^2) \cap H^1(L^3)$ we have for arbitrary $\psi \in C_0^\infty([0,T]; C_0^\infty(\Omega))$

$$
\int_0^T \int_\Omega (a_{\xi''} + a_{\xi'}') \psi \, dx \, d\sigma = \lim_{k \to \infty} \int_0^T \int_\Omega (a_{k\xi''} + a_{k\xi'}) \psi \, dx \, d\sigma
$$

$$
= \lim_{k \to \infty} \int_0^T \int_\Omega (-a_k \phi') \xi' + a_k \xi \psi \, dx \, d\sigma = -\lim_{k \to \infty} \int_0^T \int_\Omega a_k \xi \psi \, dx \, d\sigma
$$

$$
= -\int_0^T \int_\Omega a \xi' \psi' \, dx \, d\sigma.
$$

By (22) and (23) we also have

$$
\lim_{n \to \infty} \int_0^T \frac{b}{c} \int_\Gamma_n \xi'' \psi \, d\gamma \, d\sigma = \int_0^T \frac{b}{c} \int_\Gamma_n (\text{tr}\Gamma_n \xi') \psi \, d\gamma \, d\sigma. \quad (25)
$$

Now for any $\phi \in C([0,T]), i \in N$, we multiply (14) by $\phi$ and integrate over $[0,T]$. This yields for any $n \geq i$

$$
\int_0^T \{(a\xi')', w_i \} \phi \, d\sigma + (c^2 \nabla \xi + b \nabla \xi', \nabla w_i) \phi \, d\sigma + \int_0^T \int_{\Gamma_n} (c\xi'' + b\xi') w_i \, d\gamma \, d\sigma
$$

$$
= \int_0^T \int_{\Gamma_n} (c^2 g + b g') w_i \, d\gamma \, d\sigma + \int_0^T (f, w_i) \phi \, d\sigma.
$$

The preceding discussion shows that one can pass to the limit to show that $\xi$ satisfies the equation

$$
\int_0^T \{(a\xi')', w_i \} \phi \, d\sigma + (c^2 \nabla \xi + b \nabla \xi', \nabla w_i) \phi \, d\sigma + \int_0^T \int_{\Gamma_n} (c\xi'' + b\xi') w_i \, d\gamma \, d\sigma
$$

$$
= \int_0^T \int_{\Gamma_n} (c^2 g + b g') w_i \, d\gamma \, d\sigma + \int_0^T (f, w_i) \phi \, d\sigma,
$$

(27)

which holds for all $i \in N$ and all $\phi \in C([0,T])$. Since the elements $w_i$ span $H^1(\Omega)$, we conclude that for any $v \in H^1(\Omega)$

$$
\int_0^T \{(a\xi')', v \} \phi \, d\sigma + (c^2 \nabla \xi + b \nabla \xi', \nabla v) \phi \, d\sigma + \int_0^T \int_{\Gamma_n} (c\xi'' + b\xi') v \, d\gamma \, d\sigma
$$

$$
= \int_0^T \int_{\Gamma_n} (c^2 g + b g') v \, d\gamma \, d\sigma + \int_0^T (f, v) \phi \, d\sigma.
$$

(28)

Next we discuss the initial condition for $\xi$. In view of $\xi_n \to \xi$ strongly in $C(L^2)$ we deduce

$$
\xi(0) = \lim_{n \to \infty} \xi_n(0) = \lim_{n \to \infty} \xi_n^0 = \xi_0 \text{ in } L^2(\Omega).
$$

Since $\xi \in H^2(L^2) \subseteq C^1(L^2)$ we can conclude that $\xi'(0)$ exists in $L^2(\Omega)$. For any $\phi \in C^1([0,T])$ such that $\phi(T) = 0$, integration by parts in the first term of (26) gives

$$
\int_0^T ((a\xi_n')', w_i) \phi \, d\sigma = -(a(0)\xi_1^n, w_i) \phi(0) - \int_0^T ((a\xi_n'), w_i) \phi' \, d\sigma
$$
Inserting this into (26) and passing to the limit results in

\[- (a(0)\xi_1, w_i)\phi(0) - \int_0^T \{((a\xi'), w_i)\phi' - (c^2\nabla \xi + b\nabla \xi', \nabla w_i)\phi\} \, d\sigma \]

\[+ \int_0^T \int_{\Gamma_n} (c\xi' + \frac{b}{c} \xi'') w_i \, d\gamma \, d\sigma = \int_0^T \int_{\Gamma_n} (c^2 g + bg') w_i \, d\gamma \, d\sigma + \int_0^T (f, w_i) \, d\sigma,\]

Integrating by parts in (27) leads to

\[- (a(0)\xi'(0), w_i)\phi(0) - \int_0^T \{((a\xi'), w_i)\phi' - (c^2\nabla \xi + b\nabla \xi', \nabla w_i)\phi\} \, d\sigma \]

\[+ \int_0^T \int_{\Gamma_n} (c\xi' + \frac{b}{c} \xi'') w_i \, d\gamma \, d\sigma = \int_0^T \int_{\Gamma_n} (c^2 g + bg') w_i \, d\gamma \, d\sigma + \int_0^T (f, w_i) \, d\sigma,\]

Therefore

\[a(0)\xi_1, w_i) = (a(0)\xi'(0), w_i)\]

holds for all \(i \in \mathbb{N}\). Since \(\{w_i : i \in \mathbb{N}\}\) is dense in \(H^1(\Omega)\) which itself is dense in \(L^2(\Omega)\) we conclude that

\[a(0)\xi_1, v) = (a(0)\xi'(0), v)\]

holds for all \(v \in L^2(\Omega)\) which considering \(a(0) \geq \frac{1}{2}\) implies

\[\xi'(0) = \xi_1.\]

The pointwise bounds in (20) together with (21) can be interpreted in the sense that \(\xi_n(s)\) and \(\xi'_n(s)\) are bounded in \(L^\infty(H^1) = (L^1(H^1)^*)^*\). Thus there exists a subsequence and elements \(z, \tilde{z} \in L^\infty(H^1)\) such that

\[\xi_n \rightharpoonup^* z, \quad \xi'_n \rightharpoonup^* \tilde{z}.\]

In view of \(\xi_n \rightharpoonup \xi\) in \(L^2(H^1)\) (cf. (22)) we conclude \(z = \xi\). To show that also \(\tilde{z} = \xi'\) holds, for arbitrary \(v \in H^1(\Omega), \phi \in C_0^\infty(0, T)\) we infer \(\phi \otimes v \in L^1(H^1)\) and therefore

\[\lim_{n \to \infty} \int_0^T \langle \xi'_n, v \rangle_{H^1(\Omega)} \phi \, d\sigma = \int_0^T \langle \tilde{z}, v \rangle_{H^1(\Omega)} \phi \, d\sigma = \int_0^T \langle \tilde{z} \phi \, d\sigma, v \rangle_{H^1(\Omega)}\]

On the other hand

\[\lim_{n \to \infty} \int_0^T \langle \xi'_n, v \rangle_{H^1(\Omega)} \phi \, d\sigma = \lim_{n \to \infty} \int_0^T \langle \xi'_n \phi \, d\sigma, v \rangle_{H^1(\Omega)}\]

\[= - \lim_{n \to \infty} \int_0^T \langle \xi_n \phi' \, d\sigma, v \rangle_{H^1(\Omega)} = - \lim_{n \to \infty} \int_0^T \langle \xi_n, v \rangle_{H^1(\Omega)} \phi' \, d\sigma\]

\[= - \int_0^T \langle \xi, v \rangle_{H^1(\Omega)} \phi' \, d\sigma = - \langle \int_0^T \xi \phi' \, d\sigma, v \rangle_{H^1(\Omega)}\]

Hence

\[\langle \int_0^T \tilde{z} \phi \, d\sigma, v \rangle_{H^1(\Omega)} = - \langle \int_0^T \xi \phi' \, d\sigma, v \rangle_{H^1(\Omega)}, \quad v \in H^1\]

and therefore

\[\int_0^T \tilde{z} \phi \, d\sigma = - \int_0^T \xi \phi' \, d\sigma\]

which implies

\[\tilde{z} = \xi'.\]

Thus we also obtain \(\xi' \in L^\infty(H^1)\), hence \(\xi\) satisfies the regularity (7) and the a priori bound (9).
Since (28) holds for all \( \phi \in C([0, T]) \) and the integrand
\[
((a \xi')', v) + (c^2 \nabla \xi + b \nabla \xi', \nabla v) + \int_{\Gamma_n} (e^{\xi'} + \frac{b}{c} (\text{tr}_{\Gamma_n} \xi')') v \, d\gamma - \int_{\Gamma_n} (c^2 g + bg') v \, d\gamma - (f, v)
\]
defines a function in \( L^2(0, T) \) for \( v \in H^1(\Omega) \), we deduce that \( \xi \) solves (13), i.e., (6) has a weak solution with the additional regularity (7).

The a priori estimate (9) ensures the uniqueness of the solution due to linearity and the fact that the right hand side vanishes for vanishing data. Therefore not only the subsequence but also the original sequence of Galerkin approximations \( (\xi_n)_{n \in \mathbb{N}} \) converges to \( \xi \) in the sense of (22).

**Step 5. higher spatial regularity.** Inserting \( v \in C^\infty_0(\Omega) \) into (13) implies
\[
((a \xi')', v) + (c^2 \nabla \xi + b \nabla \xi', \nabla v) = (f, v), \tag{29}
\]
hence
\[
(a \xi')' - c^2 \Delta \xi - b \Delta \xi' = f \tag{30}
\]
is satisfied in the sense of distributions almost everywhere on \([0, T]\). Note that (29) implies the following ordinary differential equation for \((\Delta \xi, v) = - (\nabla \xi, \nabla v)\)
\[
(\Delta \xi, v)' + \frac{c^2}{b} (\Delta \xi, v) = \frac{1}{b} ((a \xi')' - f, v)
\]
\[
(\Delta \xi(0), v) = (\Delta \xi_0, v)
\]
whose solution is given by
\[
(\Delta \xi, v)(\sigma) = (\Delta \xi(\sigma), v) = e^{-\frac{c^2}{b} \sigma} (\Delta \xi_0, v) + \frac{1}{b} \int_0^\sigma e^{-\frac{c^2}{b} (\sigma - \tau)} ((a \xi')' - f, v) \, d\tau
\]
\[
= (e^{-\frac{c^2}{b} \sigma} \Delta \xi_0 + \frac{1}{b} \int_0^\sigma e^{-\frac{c^2}{b} (\sigma - \tau)} ((a \xi')' - f) \, d\tau, v)
\]
This justifies the identification
\[
\Delta \xi(\sigma) = e^{-\frac{c^2}{b} \sigma} \Delta \xi_0 + \frac{1}{b} \int_0^\sigma e^{-\frac{c^2}{b} (\sigma - \tau)} ((a \xi')' - f) \, d\tau \tag{31}
\]
which by (7) reveals
\[
\Delta \xi \in H^1(L^2). \tag{32}
\]

**Remark 1.** The regularity of \( \Delta \xi \) can be improved in the case \( f = 0 \) and \( \xi(0) = \xi'(0) = 0 \). Then we have
\[
\Delta \xi(\sigma) = \frac{1}{b} \int_0^\sigma e^{-\frac{c^2}{b} (\sigma - \tau)} (a \xi')' \, d\tau.
\]
Integrating by parts we obtain
\[
\Delta \xi(\sigma) = \frac{1}{b} a \xi'(\sigma) - \frac{c^2}{b^2} \int_0^\sigma e^{-\frac{c^2}{b} (\sigma - \tau)} a \xi' \, d\tau,
\]
from which together with (7) and \( a \in C^1([0, T], L^2(\Omega)) \cap W^{1, \infty}(0, T; L^3(\Omega)) \cap C([0, T], L^\infty(\Omega)) \) we deduce
\[
\Delta \xi \in L^\infty(L^6) \cap W^{1, \infty}(0, T; L^2(\Omega)). \tag{33}
\]
As a consequence of the regularity (7), (32), the PDE (30) holds in \( L^2(\Omega) \) a.e. in \([0,T]\) and \( \frac{\partial \xi'}{\partial \nu} \) exist at least in \( H^{-1/2}(\partial \Omega) \) and
\[
\frac{\partial \xi'}{\partial \nu} \in H^1(\Omega) (H^{-1/2}(\partial \Omega)).
\] (34)

By Green’s formula we find from (13) for \( v \in H^1(\Omega) \)
\[
\langle (a\xi')' - c^2 \Delta \xi = b \Delta \xi', v \rangle + \langle c^2 \frac{\partial \xi'}{\partial \nu} + b \frac{\partial \xi'}{\partial \nu}, v \rangle_{\partial \Omega}
\]
\[
+ \int_{\Gamma_a} (c\xi' + \frac{b}{c}(\text{tr}_{\Gamma_a} \xi')') v \, d\gamma = \int_{\Gamma_a} (c^2 g + bg') v \, d\gamma + (f, v), \text{ a.e. in } [0,T],
\]
where \( \langle \cdot, \cdot \rangle_{\partial \Omega} \) stands for the duality pairing between \( H^{-1/2}(\partial \Omega) \) and \( H^{1/2}(\partial \Omega) \).

Note that by (34) \( \langle c^2 \frac{\partial \xi'}{\partial \nu} + b \frac{\partial \xi'}{\partial \nu}, v \rangle_{\partial \Omega} \) makes sense and defines a function in \( L^2(0,T) \).

Then (30) entails
\[
\langle c^2 \frac{\partial \xi'}{\partial \nu} + b \frac{\partial \xi'}{\partial \nu}, v \rangle_{\partial \Omega} = - \int_{\Gamma_a} (c\xi' + \frac{b}{c}(\text{tr}_{\Gamma_a} \xi')') v \, d\gamma + \int_{\Gamma_a} (c^2 g + bg') v \, d\gamma
\]

Multiplying by \( e^{\frac{c^2}{\sigma}} \) we can write this as
\[
b(e^{\frac{c^2}{\sigma}} (\xi', \varphi)_{L^2(\Omega)})' + b e^{\frac{c^2}{\sigma}} (g, \varphi)_{L^2(\Omega)}
\]

which implies
\[
e^{\frac{c^2}{\sigma}} (\xi', \varphi)_{\partial \Omega} + \frac{1}{c} (\xi', \varphi)_{L^2(\Omega)} - (g, \varphi)_{L^2(\Omega)}
\]

(36)

Let us introduce the spaces
\[
H^{1/2}_0(\Omega) = \{ \varphi \in H^{1/2}(\partial \Omega): \exists v \in H^1(\Omega): \varphi = \text{tr}_\Gamma v \text{ on } \Omega, \varphi = 0 \text{ on } \Omega \backslash \bar{\Omega} \}
\]

where \( \Omega \in \{ \Gamma_a, \Gamma_n \} \). For \( \varphi \in H^{1/2}_0(\Gamma_a) \) we therefore find
\[
e^{\frac{c^2}{\sigma}} ((\xi', \varphi)_{\partial \Omega} + \frac{1}{c} (\xi', \varphi)_{L^2(\Omega)}) = \frac{\partial \xi'}{\partial \nu}(0), \varphi)_{\partial \Omega} + \frac{1}{c} (\xi'(0), \varphi)_{L^2(\Omega)} = 0,
\]
due to the compatibility condition (10).

This implies
\[
\frac{1}{c} (\xi'(0), \varphi)_{L^2(\Omega)} = \frac{\partial \xi'}{\partial \nu}(0), \varphi)_{\partial \Omega} = 0, \quad \varphi \in H^{1/2}_0(\Gamma_a),
\]
hence
\[
\frac{1}{c} \xi' + \frac{\partial \xi'}{\partial \nu} = 0
\]
holds in \( L^2(H^{1/2}_0(\Gamma_a)^*) \). Similarly, choosing \( \varphi \in H^{1/2}_0(\Gamma_n) \) one finds
\[
e^{\frac{c^2}{\sigma}} ((\xi', \varphi)_{\partial \Omega} - (g, \varphi)_{L^2(\Omega)}) = \frac{\partial \xi'}{\partial \nu}(0), \varphi)_{\partial \Omega} - (g(0), \varphi)_{L^2(\Omega)} = 0,
\]
by the compatibility condition (11). Thus
\[
\frac{\partial \xi'}{\partial \nu} = g
\]
holds in \( L^2(H^{1/2}_0(\Gamma_n)^*) \). Thus we have shown that the unique weak solution of (13) satisfies the strong form (6) almost everywhere in time.
Our next goal is to prove higher spatial regularity and particularly pointwise boundedness of $\xi$ by considering (32) with appropriate boundary conditions and employing elliptic regularity. In view of (31) and since $(a\xi')' \in L^2(L^2)$ we can consider for almost all $\sigma \in [0, T]$ the elliptic Neumann problem
\[
\Delta z(\sigma) = e^{-\frac{\sigma}{c}}\Delta \xi_0 + \frac{1}{b} \int_0^\sigma e^{-\frac{\tau}{c}}((a\xi')' - f) \, d\tau =: F(\sigma), \quad \text{in } \Omega
\]
\[
\frac{\partial z}{\partial \nu}(\sigma) = g(\sigma), \quad \text{on } \Gamma_n, \quad (37)
\]
\[
\frac{\partial z}{\partial \nu}(\sigma) = -\frac{1}{c}\xi'(\sigma), \quad \text{on } \Gamma_n.
\]
At first we verify the solvability condition
\[
e^{-\frac{\sigma}{c}}(\Delta \xi_0, 1) + \frac{1}{b} \int_0^\sigma e^{-\frac{\tau}{c}}((a\xi')'(\tau) - f(\tau), 1) \, d\tau
\]
\[
= -\frac{1}{c}(\xi'(\sigma), 1)_{L^2(\Gamma_a)} + (g, 1)_{L^2(\Gamma_n)}, \quad (38)
\]
Inserting $v = 1$ into (13) results in
\[
e^{\frac{\tau}{c}r}((a\xi')'(\tau) - f(\tau), 1) = -e^{\frac{\tau}{c}r}(c\xi' + \frac{b}{c}\xi'', 1)_{L^2(\Gamma_a)} + e^{\frac{\tau}{c}r}(c^2 g + bg', 1)_{L^2(\Gamma_n)}
\]
\[
= -\frac{b}{c}(e^{\frac{\tau}{c}r}\xi', 1)_{L^2(\Gamma_a)} + b(e^{\frac{\tau}{c}r}g, 1)_{L^2(\Gamma_a)} = b(e^{\frac{\tau}{c}r}(\frac{\partial g}{\partial \nu}(\tau), 1)_{\partial \Omega})',
\]
where the last equality follows from (35). Observe that by (10), (11)
\[
(\Delta \xi_0, 1) = \left(\frac{\partial \xi_0}{\partial \nu}, 1\right)_{L^2(\Gamma_a)} + \left(\frac{\partial \xi_0}{\partial \nu}, 1\right)_{L^2(\Gamma_n)}
\]
\[
= -\frac{1}{c}(\xi, 1)_{L^2(\Gamma_a)} + (g(0), 1)_{L^2(\Gamma_n)}.
\]
This together with (36) entails the solvability condition
\[
e^{-\frac{\sigma}{c}}(\Delta \xi_0, 1) + \frac{1}{b} \int_0^\sigma e^{-\frac{\tau}{c}}((a\xi')'(\tau) - f(\tau), 1) \, d\tau
\]
\[
= e^{-\frac{\sigma}{c}}\left[\frac{1}{c}(\xi, 1)_{L^2(\Gamma_a)} + (g(0), 1)_{L^2(\Gamma_n)} + e^{\frac{\tau}{c}}(\frac{\partial g}{\partial \nu}(\sigma), 1)_{\partial \Omega} - \left(\frac{\partial \xi_0}{\partial \nu}(0), 1\right)_{\partial \Omega}\right]
\]
\[
= e^{-\frac{\sigma}{c}}\left[\frac{1}{c}(\xi, 1)_{L^2(\Gamma_a)} + (g(0), 1)_{L^2(\Gamma_n)} - \left(\frac{\partial \xi_0}{\partial \nu}(0), 1\right)_{\partial \Omega}\right] + \left(\frac{\partial g}{\partial \nu}(\sigma), 1\right)_{\partial \Omega}
\]
\[
= -\frac{1}{c}(\xi'(\sigma), 1)_{L^2(\Gamma_a)} + (g(\sigma), 1)_{L^2(\Gamma_n)}.
\]
The Neumann data
\[
\varphi(\sigma) = \begin{cases} 
g(\sigma) & \text{on } \Gamma_n, 
-\frac{1}{c}\text{tr}_{\Gamma_n}\xi'(\sigma) & \text{on } \Gamma_a,
\end{cases}
\]
in general does not belong to $H^{1/2}(\partial \Omega)$ even if $g(\sigma), \text{tr}_{\Gamma_n}\xi'(\sigma)$ exhibit $H^{1/2}$ regularity on the respective boundary parts, since global $H^{1/2}$ regularity would require continuity over the interface between $\Gamma_a$ and $\Gamma_n$. Still it can be shown that $\varphi(\sigma)$ is an element of $H^s(\partial \Omega)$ for $0 < s < \frac{1}{2}$ (see [8, Corollary 1.4.4.5.] and the Appendix) and that
\[
\|\varphi(\sigma)\|_{H^s(\partial \Omega)} \leq \|\varphi(\sigma)\|_{H^s(\Gamma_n)} + \|\varphi(\sigma)\|_{H^s(\Gamma_a)}
\]
holds.
This yields
\[ \|\varphi\|_{L^\infty(H^s(\partial\Omega))}^2 \leq \|g\|_{L^\infty(H^s(\Gamma_n))}^2 + C_{\text{tr},\Gamma_n} \|\xi'\|_{L^\infty(H^s)}^2. \]

Elliptic regularity results imply that (37) admits a solution \( z(\sigma) \in H^{s+3/2}(\Omega) \) which is unique up to a constant (which may depend on \( \sigma \)). This constant is determined by the fact that \( \xi \) is a solution of (36), hence by (31) we have \( z(\sigma) = \xi(\sigma) \). Moreover, we have the estimate
\[ \|\xi(\sigma)\|_{H^{s+3/2}(\Omega)} \leq C_{\text{ell}} \left( \|F\|_{L^2(\Omega)} + \|\varphi(\sigma)\|_{H^s(\partial\Omega)} \right) \tag{39} \]
where \( F \) is determined by the right hand side in (37) and where the constant \( C_{\text{ell}} > 0 \) does not depend on \( \sigma \). Indeed, we can employ the Exact Interpolation Theorem [1, Theorem 7.23] together with boundedness of the solution operator \( S : X_i \to Y_i \), \( Sq = v, i = 1, 2 \) to the Neumann Laplace problem
\[ \begin{align*}
\Delta v &= 0, \quad \text{in } \Omega \\
\frac{\partial v}{\partial \nu} &= q, \quad \text{on } \partial\Omega \\
\int_\Omega v \, dx &= 0
\end{align*} \]
with \( X_1 = H^{-1/2}(\partial\Omega), Y_1 = H^1(\Omega), X_2 = H^{1/2}(\partial\Omega), Y_2 = H^2(\Omega) \) to conclude that \( S \) is also bounded between the interpolated spaces \( X_s = H^s(\partial\Omega) \) and \( Y_s = H^{3/2+s}(\Omega) \). The estimate (39) then follows by decomposition of \( \xi \) as \( \xi(\sigma) = S\varphi(\sigma) + \xi_F(\sigma) \), where \( \xi_F(\sigma) \) solves (37) with homogeneous Neumann boundary conditions (and a \( \sigma \) dependent constant such that (36) is satisfied).

Since \( H^{s+3/2}(\Omega) \) embeds continuously into \( C(\Omega) \) with constant \( C_{\Omega,s+3/2} \) we obtain the estimate
\[ \|\xi\|_{L^\infty(C(\Omega))} \leq C_{\Omega,s+3/2} C_{\text{ell}} \left( \|F\|_{L^\infty(L^2(\Omega))} + \|\varphi\|_{L^\infty(H^s(\partial\Omega))} \right) \]
Using (12), one can verify the estimate
\[ \|F\|_{L^\infty(L^2(\Omega))} \leq \|\Delta \xi_0\|_{L^2(\Omega)} + \frac{3}{2b} \|\xi''\|_{L^1(L^2)} + \frac{\|a'\|_{L^\infty(L^3)}}{b} \|\xi'\|_{L^1(L^6)} + \frac{1}{b} \|f\|_{L^1(L^2)} \]
Combining the above estimates with (9) and (21) one eventually finds
\[ \|\xi\|_{L^\infty(C(\Omega))}^2 \leq C_3 \left( 1 + T \right) \left( 1 + \|a'\|_{L^\infty(L^3)} \right)^2 \left( \|\Delta \xi_0\|_{L^2(\Omega)}^2 + \|\xi_0\|^2_{H^1(\Omega)} + \|\xi_1\|^2_{H^1(\Omega)} \right) \]
\[ + \|c^2 g + b g'\|_{H^1(H^{-1/2}(\Gamma_n))} + \|g\|_{L^\infty(H^{-1}(\Gamma_n))} \]
\[ + \|f\|_{L^2((H^1)^*)}^2 + \|f\|_{L^1(L^2)}^2 + \|f'\|_{L^2((H^1)^*)}^2 \] \tag{40} \]

**Theorem 2.** Under assumptions \((H1)-(H4)\) the Westervelt equation (5) has a unique solution \( u \) in
\[ \begin{align*}
H^2(0, T; L^2(\Omega)) \cap W^{1,\infty}(0, T; H^1(\Omega)) &\cap H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^{3/2+s}(\Omega)) \\
&\subseteq L^\infty(0, T; C(\Omega))
\end{align*} \]
provided
\[ r_0^2 = \|\Delta u_0\|_{L^2(L^2)}^2 + \|u_0\|_{H^1(\Omega)}^2 + \|u_1\|_{H^1(\Omega)}^2 + \|c^2 g + b g'\|_{H^1(H^{-1/2}(\Gamma_n))}^2 + \|g\|_{L^\infty(H^{-1}(\Gamma_n))}^2 \]
is sufficiently small. The solution \( u \) satisfies the a priori estimates
\[
\|u\|_{L^3}^2 \leq C_4(1 + T) \left( \|u_0\|_{L^2(\Omega)}^2 + \|u_1\|_{H^1(\Omega)}^2 + \|c^2 g + bg'\|_{L^\infty(H^{-1/2}(\Gamma_n))^2} + \|c^2 g + bg'\|_{H^1(\Gamma_n)}^2 \right),
\]
with \( X \) as in (7)
\[
\|u\|^2_{L^\infty(0, T; C(\overline{\Omega}))} \leq C_5(1 + T) \left( \|\Delta u_0\|_{L^2(\Omega)}^2 + \|g\|_{L^\infty(0, T; H^s(\Gamma_n))} + \|u_0\|_{H^1(\Omega)}^2 \right) + \|u_1\|_{H^1(\Omega)}^2 + \|c^2 g + bg'\|_{L^\infty(H^{-1/2}(\Gamma_n))^2} + \|c^2 g + bg'\|_{H^1(\Gamma_n)}^2,
\]
(41) (42)

Proof. We have shown that for every \( y \) satisfying the assumptions of Theorem 1 the linearized system (6) has a unique solution \( \xi = Ty \). In view of
\[
((1 - ku)u)'' = ((1 - 2ku)u')'
\]
it is clear that a fixed point of \( T \) is a solution of (5). We now verify the assumptions of the contraction mapping principle. Let \( y \) and \( \dot{y} \) satisfy the assumptions of Theorem 1 and denote the corresponding solutions by \( \xi \) and \( \dot{\xi} \). Then the difference \( z = \xi - \dot{\xi} \) satisfies
\[
((az')', v) + (c^2 \nabla z + b \nabla z', \nabla v) + \int_{\Gamma_n} (cz' + \frac{b}{c} z'')v\,d\gamma
= -((\langle \xi' \rangle, v), v) + \int_{\Gamma_n} (c\xi' + \frac{b}{c} \xi'')v\,d\gamma
= -((\langle \xi' \rangle, v), v) + \int_{\Gamma_n} (c\xi' + \frac{b}{c} \xi'')v\,d\gamma
\]
(43)
\[
z(0) = 0, \quad z'(0) = 0,
\]
where \( \tilde{a} = 1 - 2k\dot{y} \). Since the right hand side of this equation just belongs to \( L^2((H^1(\Omega))^*) \), we can only use the lower order energy estimate (8) to obtain
\[
\|z'(s)\|^2_{L^2(\Omega)} + \|\nabla z(s)\|^2_{L^2(\Omega)} + \|\xi'(s)\|^2_{L^2(\Gamma_n)} + \int_0^s \|z'\|^2_{H^1(\Omega)}\,d\sigma
\]
\[
\leq C_1 \|((\tilde{a} - a)\dot{\xi}')\|^2_{L^2((H^1(\Omega))^*)},
\]
(44)
For almost all \( \sigma \in [0, T] \) we obtain
\[
\|((\tilde{a} - a)\dot{\xi}')\|_{H^1(\Omega)} = \sup_{\|v\|_{H^1(\Omega)} \leq 1} \langle ((\tilde{a} - a)\dot{\xi}')(\sigma), v \rangle
\]
\[
= \sup_{\|v\|_{H^1(\Omega)} \leq 1} \langle ((\tilde{a} - a)(\sigma)\dot{\xi}'(\sigma) + ((\tilde{a} - a)(\sigma)\dot{\xi}'(\sigma), v)\rangle.
\]
Since \( \dot{\xi}'(\sigma) \in L^2(\Omega) \), \( (\tilde{a} - a)(\sigma) \in L^3(\Omega) \), for any \( v \in H^1(\Omega) \) one finds
\[
\|((\tilde{a} - a)(\sigma)\dot{\xi}'(\sigma), v)\| \leq C_{1,6} \|((\tilde{a} - a)(\sigma)\dot{\xi}'(\sigma), v)\| L^3(\Omega) \|\dot{\xi}'(\sigma)\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)}.
\]
Similarly one obtains
\[
\|((\tilde{a} - a)(\sigma)\dot{\xi}'(\sigma), v)\| \leq C_{1,6,3} \|((\tilde{a} - a)(\sigma)\dot{\xi}'(\sigma), v)\| L^3(\Omega) \|\dot{\xi}'(\sigma)\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)},
\]
which leads to
\[
\|((\tilde{a} - a)\dot{\xi}')\|^2_{L^2((H^1(\Omega))^*)}
\]
\[
\leq \|\dot{\xi}''\|^2_{L^2(L^2(\Omega))} + \|\dot{\xi}'\|^2_{L^2(L^2(\Omega))} (C_{1,6} \|\tilde{a} - a\|^2_{L^2(L^2(\Omega)))} + C_{1,6,3} \|((\tilde{a} - a)'\|^2_{L^2(L^2(\Omega)))}.
\]
Combining this estimate with (44) and
\[
\|z(s)\|^2_{L^2(\Omega)} \leq T \int_0^s \|z'\|^2_{L^2(\Omega)}\,d\sigma,
\]
one can in particular derive the estimate
\[ \|\cdot\|_{H^1(\Omega)} \leq 8k^2 C_{\Omega, \theta} C_{\Omega, \delta} C_1 (1 + T)(\|\xi''\|_{L^2(\Omega)} + \|\xi''\|_{L^2(\Omega)}) \|\eta - 2\|_{H^1(\Omega)}. \] (45)
This suggests to work with the Banach space
\[ \hat{X} := H^1(\Omega). \]
Then, provided \( y \) satisfies the conditions of the first part of Theorem 1, i.e., \( y \in C^1([0, T], L^2(\Omega)) \cap W^{1, \infty}(0, T; L^2(\Omega)) \cap C([0, T], L^\infty(\Omega)), \|y\|_{L^\infty(0, T; L^\infty(\Omega))} \leq \frac{1}{16}, \]
\( \|y''\|_{L^\infty(0, T; L^2(\Omega))} \leq \frac{\min(b, c)}{4kC_{\Omega, \delta}}, \) estimate (45) and the a priori estimate (9) with (21) give rise to
\[ \|\mathcal{T}y - Ty\|_X^2 \leq 8k^2 C_{\Omega, \theta} C_{\Omega, \delta} C_1 (1 + T)(\|\mathcal{T}y''\|_{L^2(\Omega)} + \|\mathcal{T}y''\|_{L^2(\Omega)}) \|\eta - 2\|_X^2 \]
\[ \leq \|\eta - 2\|_X^2 \frac{c}{16} (1 + T)(1 + \|y''\|_{L^\infty(\Omega)}) \cdot (\|u_0\|_{H^1(\Omega)}^2 + \|u_1\|_{H^1(\Omega)}^2 + \|c^2 g + bg'\|_{H^1(\Omega)}^2) \]
which shows that \( \mathcal{T} \) is a contraction if we impose some fixed bound \( r > 0 \) on \( \|\eta\|_{L^\infty(\Omega)} \) and if
\[ \|u_0\|_{H^1(\Omega)}^2 + \|u_1\|_{H^1(\Omega)}^2 + \|c^2 g + bg'\|_{H^1(\Omega)}^2 \]
is sufficiently small. This argument suggests to define the set
\[ W = \{ \varphi \in \hat{X} \cap L^\infty(\Omega) \cap W^{1, \infty}(\Omega): \]
\[ \|\varphi\|_{L^\infty(\Omega)} \leq \frac{1}{4k}, \|\varphi'\|_{L^\infty(\Omega)} \leq \frac{\min(b, c)}{4kC_{\Omega, \delta}}, \|\varphi'\|_{L^\infty(\Omega)} \leq r \}. \]
as the domain of the fixed point operator \( \mathcal{T} \). For \( y \in W \) the a priori bounds (9), (21) and (40) imply
\[ \|\mathcal{T}y\|_{L^\infty(\Omega)}^2 + \|\mathcal{T}y\|_{W^{1, \infty}(\Omega)}^2 \leq (C_2 + C_3)(1 + T)(1 + r^2)r_0, \]
provided additionally \( \|u_0\|_{H^2} \) is sufficiently small. Hence by boundedness of the embedding \( H^1(\Omega) \rightarrow L^2(\Omega) \), the set \( W \) is invariant under \( \mathcal{T} \) if \( r_0 \) is sufficiently small.

In order to show that \( W \) is closed in \( \hat{X} \) we chose a sequence \( (\varphi_n) \subset W \) which converges to some \( \varphi \in \hat{X} \) with respect to the \( \hat{X} \) norm. Since the \( L^\infty(\Omega) \) norm of \( \varphi \) and the \( L^\infty(\Omega) \) norm of \( \varphi' \) are bounded by \( \frac{1}{4k}, \frac{\min(b, c)}{4kC_{\Omega, \delta}}, \) and \( r \), respectively, and these norms correspond to spaces that are dual to separable spaces, there exists a subsequence, again denoted by \( (\varphi_n) \), such that \( \varphi_n \rightharpoonup \psi \) in \( L^\infty(\Omega), \varphi_n \rightharpoonup \chi \) in \( L^\infty(\Omega) \) and in \( L^\infty(\Omega) \). By uniqueness of limits we have \( \psi = \varphi \) and \( \chi = \varphi' \) and by the Banach Alaoglu Theorem (stating that balls in duals of separable spaces are weak* compact) we have \( \varphi \in W \).

Hence \( W \) is closed in \( \hat{X} \) and \( \mathcal{T} \) has a unique fixed point in \( W \). Theorem 1 yields the additional regularity \( u \in H^2(0, T; L^2(\Omega)) \cap W^{1, \infty}(0, T; H^1(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^{\frac{5}{2} + s}(\Omega)) \subseteq L^\infty(0, T; C(\Omega)), \) and the a priori estimates follow from (9), (40).

3. Preliminaries for computing the shape derivative of \( J \). Following [6, 9, 12], we construct a family of perturbations \( \Omega_t \) of a reference domain \( \Omega \in C^{1, 1}, \Omega \subset U \), by perturbing the identity with a vector field \( h \) from the set
\[ \mathcal{D} = \{ h \in C^{1, 1}(\bar{U})^2: h|_{\partial U} = 0, h|_{\Gamma_n} = 0 \}. \] (46)
For $h \in \mathcal{D}$ and $t \in \mathbb{R}$ sufficiently small define

\[ F_t = \text{id} + th, \]
\[ \Omega_t = F_t(\Omega), \quad \Gamma_t = F_t(\Gamma). \]

Then $F_t$ is a $C^{1,1}$-diffeomorphism which preserves the regularity of $\Omega$. One defines the Eulerian derivative of $J$ by

\[ dJ(\Omega)h = \lim_{t \to 0} \frac{1}{t}(J(u_t, \Omega_t) - J(u, \Omega)), \tag{47} \]

where $u$ and $u_t$ satisfy the PDE on the original and on the perturbed domain, respectively

\[ E(u, \Omega) = 0, \quad E(u_t, \Omega_t) = 0. \]

The constraint $E(u, \Omega) = 0$ stands for the weak form of the PDE with initial and boundary conditions, which is in our case

\[
\begin{aligned}
((1 - 2ku)u', v) + (c^2 \nabla u + b \nabla u', \nabla v) + \int_{\Gamma_n} (cu' + b'u'')v d\gamma \\
= \int_{\Gamma_n} (c^2 g + bg')v d\gamma, \quad v \in H^1(\Omega), \quad \sigma \in (0, T)
\end{aligned}
\tag{48}
\]

\[ u(0) = u_0, \quad u'(0) = u_1. \]

The expression $dJ(\Omega)$ is called shape derivative of $J$ if $dJ(\Omega)h$ exists for all $h \in \mathcal{D}$ and $dJ(\Omega) \in \mathcal{D}^*$. From the Delfour-Hadamard-Zolesio structure theorem we expect a representation of the form

\[ dJ(\Omega)h = \int \Gamma G(s)h \cdot \nu ds \]

to hold, which we will indeed establish in Theorem 8 below. The difficulty ensuing from the fact that the difference quotient in (47) involves functions defined on different domains can be overcome with the method of mapping. Let

\[ \varphi_t : \Omega_t \to \mathbb{R}^3 \]

then

\[ \varphi^t = \varphi_t \circ F_t : \Omega \to \mathbb{R}^3, \quad \varphi_0 = \varphi^0 : \Omega \to \mathbb{R}^3. \]

For convenience we recall some rules for differentiation and integration of the mapped functions, see, e.g., [6].

**Lemma 3.**

1. $\varphi_t \in H^1(\Omega_t)$ iff $\varphi^t \in H^1(\Omega)$ and

\[ (\nabla \varphi_t) \circ F_t = M_t \nabla \varphi^t, \]

with $M_t = DF_t - T$.

2. If $\varphi_t \in L^1(\Omega_t)$, then $\varphi^t \in L^1(\Omega)$ and

\[ \int_{\Omega_t} \varphi_t dx = \int_{\Omega} \delta_t \varphi^t dx, \]

where $\delta_t = \det(DF_t) = \det(I + t \nabla h^T)$.

3. If $\varphi_t \in L^1(\Gamma_t)$, then $\varphi^t \in L^1(\Gamma)$ and we have

\[ \int_{\Gamma_t} \varphi_t d\gamma = \int_{\Gamma} \omega_t \varphi^t d\gamma, \]

with $\omega_t = \delta_t |M_t\nu|$. 
Theorem 2 have a unique solution \( u \) on \( \Gamma \) bounds also apply to the family of transformed solutions \( u \) for \( u \) that difference equation (5) defined on \( \Omega \). The first part of the Theorem is a straightforward consequence of the fact Proof.

4. If \( f \in C((-\tau, \tau), W^{2,1}(U)) \) and \( f_0(0) \) exists in \( W^{1,1}(U) \), then

\[
\frac{d}{dt} \int_{\Gamma_t} f(t, s) \, ds \bigg|_{t=0} = \int_{\Gamma} \left\{ f_0(0, s) + \left( \frac{\partial}{\partial \nu} f(0, s) + \kappa f(0, s) \right) (h \cdot \nu) \right\} \, ds
\]

**Lemma 4.** For \( \delta_t, M_t, \omega_t \) as in Lemma 3 and \( A_t = \delta_t M_t^T M_t \) we have

\[
\lim_{t \to 0} \delta_t = \delta_0 = 1, \quad \lim_{t \to 0} \omega_t = \omega_0 = 1, \quad \lim_{t \to 0} M_t = M_0 = I,
\]

\[
\dot{\delta}_t = \frac{d\delta_t}{dt} \bigg|_{t=0} = \text{div} \, h,
\]

\[
\dot{M}_t = \frac{dM_t}{dt} \bigg|_{t=0} = -\nabla h,
\]

\[
\dot{A}_t = \frac{dA_t}{dt} \bigg|_{t=0} = A = \text{div} \, hI - \nabla h - (\nabla h)^T,
\]

\[
\omega_t = \frac{d\omega_t}{dt} \bigg|_{t=0} = \text{div}_\Gamma \, h = \text{div} \, h|_{\Gamma} - \nabla h \nu \cdot \nu.
\]

Replacing \( \Omega \) by \( \Omega_t \) in (48) defines a family of perturbed problems which by Theorem 2 have a unique solution \( u_t \in L^\infty(0, T; L^\infty(\Omega_t)) \cap H^2(0, T; L^2(\Omega_t)) \cap W^{1,\infty}(0, T; H^1(\Omega_t)) \). Using the above transformation rules and observing \( \delta_t \equiv 1 \) on \( \Gamma \), one can verify that the transformed solution \( u^t \) satisfies

\[
((1 - 2ku^t)(u^t)'', \delta_t v) + (A_t(c^2 \nabla u^t + b(\nabla u^t)', \nabla v) + \int_{\Gamma_u} (c(u^t)' + b(c^2(u^t)'') v \, d\gamma
\]

\[
= \int_{\Gamma_u} (c^2 g^t + b(g^t)') \omega_t v \, d\gamma, \quad v \in H^1(\Omega), \quad \sigma \in (0, T),
\]

\[
u^t(0) = u_0^t, \quad (u^t)'(0) = u_1^t.
\]

**Theorem 5.** Equation (49) has a unique solution

\( u^t \in L^\infty(0, T; L^\infty(\Omega)) \cap H^2(0, T; L^2(\Omega)) \cap W^{1,\infty}(0, T; H^1(\Omega)) \)

for \( t \) sufficiently small. This family of solutions satisfies the a priori bounds (41) and (42) uniformly in \( t \). Moreover we have for \( u_0, u_1 \) and \( g \) sufficiently small

\[
\lim_{t \to 0} \frac{1}{t} \| u^t - u \|_X^2 = 0,
\]

(50)

where \( u \) is the solution of (5) and

\( \bar{X} := \{ \phi \in W^{1,\infty}(0, T; L^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) : \text{tr} \phi' \in L^\infty(0, T; L^2(\Gamma_u)) \} \)

Proof. The first part of the Theorem is a straightforward consequence of the fact that \( u^t \) is the diffeomorphic image of the corresponding solution of the Westervelt equation (5) defined on \( \Omega_t \). Since the constants appearing in the a priori estimates for \( u_t \) can be bounded uniformly with respect to \( t \) one can argue that the a priori bounds also apply to the family of transformed solutions \( u^t \) for \( t \) sufficiently small.

Next we turn to the analysis of the dependence of \( u^t \) on \( t \). Let \( z^t \) stand for the difference

\[
z^t = \frac{1}{\sqrt{t}} (u^t - u^0) = \frac{1}{\sqrt{t}} (u^t - u).
\]
Subtracting (48) from (49) one can verify that $z^t$ satisfies the equation

$$
((1 - 2ku)(z^t)'', v) + (c^2 \nabla z^t + b \nabla (z^t)', \nabla v) + \int_{\Gamma_n} (c(z^t)' + \frac{b}{c}(z^t)''v \, d\gamma
$$

$$= 2k((u^t)'z^t)'', v) - \left( \frac{\delta_t - 1}{\sqrt{t}} ((1 - ku^t)u^t)'', v \right) - \left( \frac{A_t - I}{\sqrt{t}} (c^2 \nabla u^t + b \nabla (u^t)') \nabla v \right)
$$

$$+ \int_{\Gamma_n} \omega_t - \frac{1}{\sqrt{t}} (c^2 g^t + b(g^t)') v \, d\gamma + \int_{\Gamma_n} \left( c^2 g^t - g \right) \frac{g'}{\sqrt{t}} v \, d\gamma,
$$

$$z^t(0) = \frac{u_0^t - u_0}{\sqrt{t}}, \quad (z^t)'(0) = \frac{u_1^t - u_1}{\sqrt{t}},
$$

(51)

i.e., the weak form (13) of (6) with

$$y = u
$$

$$(f, v) = 2k((u^t)'z^t)'', v - \left( \frac{\delta_t - 1}{\sqrt{t}} ((1 - ku^t)u^t)'', v \right) - \left( \frac{A_t - I}{\sqrt{t}} (c^2 \nabla u^t + b \nabla (u^t)') \nabla v \right)
$$

and $c^2 g + bg'$ replaced by

$$\tilde{g} = \frac{\omega_t - 1}{\sqrt{t}} (c^2 g^t + b(g^t)') + \left( c^2 g^t - g \right) \frac{g'}{\sqrt{t}}.
$$

By Theorem 2, the assumptions of Theorem 1 are satisfied, hence estimates (8) and (21) yield

$$\|z^t\|^2_{L^\infty(L^2(\Omega))} + \|z^t\|^2_{H^1(\Omega)} + \|\text{tr}_{\Gamma_n}(z^t)'\|^2_{L^\infty(L^2(\Gamma_n))} + \|(z^t)''\|^2_{L^2(H^1(\Omega))}
$$

$$\leq 8C_1(1 + T) \left( \left\| \frac{u_0^t - u_0}{\sqrt{t}} \right\|^2_{H^1(\Omega)} + \left\| \frac{u_1^t - u_1}{\sqrt{t}} \right\|^2_{H^1(\Omega)}
$$

$$+ \|\tilde{g}\|^2_{L^2((\Gamma_n))} + \|f\|^2_{L^2((\Gamma_n))} \right).
$$

(52)

Here we can estimate

$$\int_0^T \left\| \int_{\Gamma_n} \frac{\omega_t - 1}{\sqrt{t}} (c^2 g^t + b(g^t)') v \, d\gamma \right\|^2 \, d\sigma
$$

$$\leq \frac{\|\omega_t - 1\|^2_{L^\infty(\Omega)}}{t} \|c^2 g^t + b(g^t)\|^2_{L^2(L^{1/3}(\Gamma_n))} C^2_{F_n,4} \|v\|^2_{H^{1/2}(\Gamma_n)}
$$

$$\int_0^T \left\| \int_{\Gamma_n} \left( c^2 g^t - g \right) \frac{g'}{\sqrt{t}} v \, d\gamma \right\|^2 \, d\sigma
$$

$$\leq \frac{\|c^2 g^t + b(g^t)\|^2_{L^2(L^{1/3}(\Gamma_n))}}{t} C^2_{F_n,4} \|v\|^2_{H^{1/2}(\Gamma_n)}
$$
for any $v \in H^{1/2}(\Gamma_n)$ and
\[
\int_0^T \left| \left( \frac{\partial}{\partial t} - \frac{1}{\sqrt{t}} \right) ((1 - ku^t)u^t)', v \right|^2 \, d\sigma \\
\leq \frac{\|\delta_1 - 1\|_{L^\infty(\Omega)}^2}{t} \left( \|1 - 2ku^t\|_{L^\infty(\Omega)}^2 \|u^t\|_{L^2(\Omega)}^2 + 4k^2C_{|\Omega|}^4 \|u^t\|^2_{L^2(\Omega)} \right)
\]

where
\[
\int_0^T \left| \left( \frac{\partial}{\partial t} - \frac{1}{\sqrt{t}} \right) (c^2 \nabla u^t + b \nabla (u^t)'), \nabla v \right|^2 \, d\sigma \\
\leq \frac{\|\delta_1 - 1\|_{L^\infty(\Omega)}^2}{t} \max(c^2, b)^2 \|u^t\|^2_{H^1(\Omega)} \|v\|^2_{H^1(\Omega)}
\]

for any $v \in H^1(\Omega)$. Hence, provided $\|u_0\|^2_{H^1(\Omega)}$, $\|u_1\|^2_{H^1(\Omega)}$, $\|c^2g + bg'\|^2_{L^\infty(\Gamma_n)}$, $\|c^2g + bg'\|^2_{H^{1/2}(\Gamma_n)}$ are sufficiently small and therewith, by (41),
\[
\max\{\|u^t\|_{L^\infty(\Omega)}, \|u^t\|_{L^2(\Omega)} \} \leq \frac{1}{64k^2C_{|\Omega|}^4C_1(1 + T)},
\]
we get (50) from (52).

Finally, we provide an identity that will be used in the analysis in the next section.

**Lemma 6.** For $u, v \in \mathcal{M}$ where $\mathcal{M}$ is the linear space induced by the norm
\[
\|w\|_{\mathcal{M}} = \|w\|_{H^1(\Omega)} + \|\Delta w\|_{L^2(\Omega)} + \left\| \frac{\partial w}{\partial \nu} \right\|_{H^{s}(\partial \Omega)},
\]
for some $s \in (0, \frac{1}{2})$, the following identity holds
\[
\Phi_1(u, v) := \int_\Omega A \nabla u \cdot \nabla v = \int_\Omega (\Delta u (h \cdot \nabla v) + \Delta v (h \cdot \nabla u)) - \int_{\Gamma} \left( \frac{\partial u}{\partial \nu} (h \cdot \nabla v) + \frac{\partial v}{\partial \nu} (h \cdot \nabla u) \right) + \int_{\Gamma} \nabla u \cdot \nabla v (h \cdot \nu) =: \Phi_2(u, v)
\]
where
\[
A = I \text{div} h - \nabla h - (\nabla h)^T
\]

**Proof.** A proof of this result for $u, v \in H^2(\Omega)$ can be found in [3]. The assertion for $u, v \in \mathcal{M}$ follows from the following result on density of $C^\infty(\Omega)$ in $\mathcal{M}$. Let $\varepsilon > 0$ and $w \in \mathcal{M}$ be fixed, then we can choose $f \in C^\infty(\Omega)$, $g \in C^{0,1}(\partial \Omega) = W^{1,\infty}(\partial \Omega) \subset H^{1/2}(\partial \Omega)$ (note that the smoothness of $g$ is limited by the smoothness of $\partial \Omega$) such that
\[
\|w - \Delta w + w + f\|_{L^2(\Omega)} < c_1 \varepsilon, \quad \left\| \frac{\partial w}{\partial \nu} - g \right\|_{H^s(\partial \Omega)} < c_2 \varepsilon,
\]
(53)
with \( c_1, c_2 > 0 \) to be chosen independently of \( \varepsilon \) below. We define \( z \) as the solution to the elliptic Neumann problem
\[
-\Delta z + z = f \quad \text{in } \Omega \\
\frac{\partial z}{\partial \nu} = g \quad \text{on } \partial \Omega.
\]
Elliptic regularity and the fact that \( f \in L^2(\Omega) \), \( g \in H^{1/2}(\partial \Omega) \), yields \( z \in H^2(\Omega) \), so that we can choose \( \psi \in C^\infty(\Omega) \) such that
\[
\| z - \psi \|_{H^2(\Omega)} < c_3 \varepsilon.
\] (54)
Moreover, since the difference \( w - z \) satisfies
\[
-\Delta (w - z) + (w - z) = -\Delta w + w - f \quad \text{in } \Omega \\
\frac{\partial (w - z)}{\partial \nu} = \frac{\partial w}{\partial \nu} - g \quad \text{on } \partial \Omega,
\]
again by elliptic regularity, as well as (53), we get
\[
\| w - z \|_{H^{3/2+s}(\Omega)} < C^A_\Omega (C^{L^2\rightarrow H^{-1/2+s}}_\Omega (c_1 + c_2)) \varepsilon,
\]
where \( C^A_\Omega \) denotes the constant in the elliptic regularity estimate and \( C^{L^2\rightarrow H^{-1/2+s}}_\Omega \) the embedding constant of \( L^2(\Omega) \rightarrow H^{-1/2+s}(\Omega) \). For the difference of the Laplace operator values we get
\[
\| \Delta w - \Delta z \|_{L^2(\Omega)} = \| (w - z) - (-\Delta w + w - f) \|_{L^2(\Omega)} \
\leq C^{H^{3/2+s}\rightarrow L^2}_\Omega C^A_\Omega (C^{L^2\rightarrow H^{-1/2+s}}_\Omega (c_1 + c_2)) \varepsilon + c_1 \varepsilon,
\]
for the difference of the normal derivatives we have
\[
\| \frac{\partial w}{\partial \nu} - \frac{\partial z}{\partial \nu} \|_{H^s(\partial \Omega)} = \| \frac{\partial w}{\partial \nu} - g \|_{H^s(\partial \Omega)} < c_3 \varepsilon.
\]
These estimates together with (54) and a sufficiently small choice of \( c_1, c_2, c_3 > 0 \) yield \( \| w - \psi \|_\mathcal{M} < \varepsilon \).
Moreover, by elliptic regularity, for any \( w \in \mathcal{M} \) we have
\[
\| h \cdot \nabla w \|_{H^s(\partial \Omega)} \leq C_{tr, \partial \Omega, s} \| h \cdot \nabla w \|_{H^{1/2+s}(\Omega)} \leq C_{tr, \partial \Omega, s} \| h \|_{C^{1,1}(\Omega)} \| w \|_{H^{3/2+s}(\Omega)}
\leq C_{tr, \partial \Omega, s} \| h \|_{C^{1,1}(\Omega)} C^A_\Omega \left( C^{L^2\rightarrow H^{-1/2+s}}_\Omega (\| \Delta w + w \|_{L^2(\Omega)} + \| \frac{\partial w}{\partial \nu} \|_{H^s(\partial \Omega)}) \right)
\leq C \| w \|_\mathcal{M}.
\]
With \( \bar{u}, \bar{v} \in C^\infty(\Omega) \) such that \( \| u - \bar{u} \|_\mathcal{M} < \varepsilon, \| v - \bar{v} \|_\mathcal{M} < \varepsilon \), it is readily checked that by \( A \in L^\infty(\Omega) \) we have
\[
|\Phi_i(\bar{u}, \bar{v}) - \Phi_i(u, v)| \leq C \varepsilon, \quad i = 1, 2,
\]
for some positive constant \( C \) independent of \( \varepsilon \). Thus due to \( \Phi_1(\bar{u}, \bar{v}) - \Phi_2(\bar{u}, \bar{v}) = 0 \) we have \( |\Phi_1(u, v) - \Phi_2(u, v)| = |(\Phi_1(\bar{u}, \bar{v}) - \Phi_2(\bar{u}, \bar{v})) - (\Phi_1(\bar{u}, \bar{v}) - \Phi_1(u, v)) + (\Phi_2(\bar{u}, \bar{v}) - \Phi_2(u, v))| < 2C \varepsilon \), hence, since \( \varepsilon > 0 \) was arbitrary, \( \Phi_1(u, v) = \Phi_2(u, v) \).
\[\square\]
4. The shape derivative of $J$. In this section we turn to the sensitivity analysis of the cost functional

$$J(u, \Omega) = \int_0^T \int_\Omega (u - y_d)^2 \, dx \, d\sigma \equiv \int_0^T \int_\Omega j(u) \, dx \, d\sigma,$$

with the PDE model (5) as a constraint. In accordance with reality and to simplify the presentation we assume

$$u(0) = u'(0) = 0.$$

Furthermore we also assume that the excitation of the piezoelectric transducers on $\Gamma_n$ is determined by the trace of a globally defined function

$$g \in H^2(0, T; H^{1/2+\epsilon}(U)) \cap L^\infty(0, T; H^{1/2+\epsilon}(U))$$

for some $\epsilon \in (0, 1/2)$ and

$$y_d \in L^2(0, T; L^2(U)) \cap H^1(0, T; (H^1(U))^*)$$

Following the strategy in [9] we introduce the adjoint system

$$(1 - 2ku)p'' - c^2 \Delta p + b\Delta p' = 2(u - y_d) \equiv dj(u), \quad \text{in } (0, T) \times \Omega,$$

$$\frac{\partial p}{\partial \nu} = 0, \quad \text{on } (0, T) \times \Gamma_n,$$

$$- \frac{1}{c} p' + \frac{\partial p}{\partial \nu} = 0, \quad \text{on } (0, T) \times \Gamma_a,$$

$$p(T) = p'(T) = 0.$$

which can be written in weak form as

$$((1 - 2ku)p'', v) + (c^2 \nabla p - b\nabla p', \nabla v) + \int_{\Gamma_a} (-cp' + \frac{b}{c} p'') c \, d\gamma = (dj(u), v), \quad \text{in } (0, T) \times \Omega,$$

$$v \in H^1(\Omega),$$

$$p(T) = p'(T) = 0.$$

Reversing the time direction on can see that

$$\tilde{p}(\sigma) = p(T - \sigma)$$

satisfies

$$((1 - 2ku)\tilde{p}'', v) + (c^2 \nabla \tilde{p} - b\nabla \tilde{p}', \nabla v) + \int_{\Gamma_a} (-c\tilde{p}' + \frac{b}{c} \tilde{p}'') c \, d\gamma$$

$$= -2k(\tilde{u}'\tilde{p}', v) + (dj(\tilde{u}), v), \quad v \in H^1(\Omega),$$

$$\tilde{p}(0) = \tilde{p}(0) = 0,$$

which is the weak form (13) of the linearized system (6) considered in Section 2, with a right hand side depending on $\tilde{p}$. Hence, using Theorem (1) and a fixed point argument, one can show well-posedness of the adjoint equation.

**Corollary 7.** Under the assumptions of Theorem 2, the adjoint equation (56) has a unique solution $p \in X$ with $X$ as in (7).

**Proof.** We define the affinely linear fixed point operator $\mathcal{F}$ on an appropriate closed bounded ball $W = B^X_1(\mathcal{F}(0))$ with $r > 0$ to be chosen below, by the mapping
\( \tilde{q} \mapsto \xi = T(\tilde{q}) \), where \( \xi \) is the weak solution of (6) with \( y = \tilde{u}, g = 0, \xi_0 = 0, \xi_1 = 0, \) and \( f = f(\tilde{q}) = -2k\tilde{u}\tilde{q}' + dj(\tilde{u}) \). Indeed, due to the estimates

\[
\|f(\tilde{q})\|_{L^\infty(H^1(\Omega))} + \|f(\tilde{q})\|_{L^2((H^1(\Omega))^*)} \leq 2kC^2_{1,4} \left( \|\tilde{u}'\|_{L^\infty(L^2(\Omega))} \|\tilde{q}'\|_{L^\infty(H^1(\Omega))} + \|\tilde{u}''\|_{L^2(L^2(\Omega))} \|\tilde{q}'\|_{L^\infty(H^1(\Omega))} + 2\|u - yd\|_{L^\infty((H^1(\Omega))^*)} \right) + 2\|u - yd\|_{L^1(H^1(\Omega))}^- \leq C\|\tilde{u}\|_X \|\tilde{q}\|_X + 2\|u - yd\|_{L^\infty((H^1(\Omega))^*)} + 2\|u - yd\|_{H^1(\Omega)}^- ,
\]

and the regularity of \( u \) guaranteed by Theorem 2, we can apply Theorem 1 to conclude that for any \( \tilde{q} \in X \) we have \( T(\tilde{q}) \in X \). Moreover, since for any \( \tilde{q}_1 - \tilde{q}_2 \in X \), the difference \( \tilde{r} = T(\tilde{q}_1) - T(\tilde{q}_2) \) satisfies (6) with \( y = \tilde{u}, g = 0, \xi_0 = 0, \xi_1 = 0, \) and \( f = f(\tilde{q}_1, \tilde{q}_2) = -2k\tilde{u}'(\tilde{q}_1' - \tilde{q}_2') \), we get from (9) and (21), as well as estimates of \( T(\tilde{q}_1, \tilde{q}_2) \) similar to (57), the contractivity estimate

\[
\|T(\tilde{q}_1) - T(\tilde{q}_2)\|_X \leq 16C^2(1 + T)(1 + \|\tilde{u}'\|_{L^\infty(L^2)})C^2\|\tilde{u}\|_X \|\tilde{q}_1 - \tilde{q}_2\|_X = c^2\|\tilde{q}_1 - \tilde{q}_2\|_X
\]

with \( c < 1 \) by (41), provided \( \|u_0\|_{H^1(\Omega)}, \|u_1\|_{H^1(\Omega)}, \|c^2g + bg'\|_{L^\infty(H^{-1/2}(\Gamma_n))}, \|c^2g + bg'\|_{H^{-1/2}(\Gamma_n)} \) are sufficiently small. This contractivity estimate also yields invariance of \( T \) on \( W = B_{r^X}(0) \) with \( r = \frac{1}{1 - c} \|T(0)\|_X \). Namely for any \( \tilde{q} \) with \( \|\tilde{q} - T(0)\|_X \leq r \) we have

\[
\|T(\tilde{q}) - T(0)\|_X \leq c\|\tilde{q} - 0\|_X \leq c\|\tilde{q} - T(0)\|_X + c\|T(0)\|_X \leq r.
\]

\( \square \)

For further reference we note that the state \( u^t \) and \( p \) also satisfy the integrated equations

\[
\int_0^T \left\{ \left\{ ((1 - ku^t)u^t)'', \delta t, \phi \right\} + (A_t(c^2\nabla u^t + b\nabla (u^t)'), \nabla \phi \right\}
\]

\[
\quad + \int_{\Gamma_a} (c(u^t)'' + \frac{b}{c}(u^t)'') \phi d\gamma \right\}
\]

\[
\quad - \int_{\Gamma_a} \left( c^2 g' + (g')' \phi \right) d\gamma d\sigma \right\}
\]

\[
\quad + \int_{\Gamma_a} \left( c^2 \phi \right) d\gamma d\sigma \right\}
\]

\[
\quad + \int_{\Gamma_a} \left( c^2 \phi \right) d\gamma d\sigma \right\}
\]

\[
\quad + \int_{\Gamma_a} \left( c^2 \phi \right) d\gamma d\sigma \right\}
\]

\[
\quad - \int_{\Gamma_a} \left\{ ((1 - 2ku)p'', \phi) + (c^2\nabla p - b\nabla p', \nabla \phi) + \int_{\Gamma_a} \left( -cp' + \frac{b}{c}p'' \right) \phi d\gamma \right\}
\]

\[
\quad + \int_{\Gamma_a} \left( dj(u), \phi \right) d\sigma, \quad \phi \in L^2(0, T; H^1(\Omega)),
\]

\[
p(T) = p'(T) = 0.
\]

Note that \( u \) satisfies (58) with \( t = 0 \).
Theorem 8. Let the assumptions made in this section hold. Then the shape derivative of \( J \) exists for any vector field \( h \in \mathcal{D} \) and is given by

\[
dJ(\Omega)h = \int_0^T \int_{\Gamma_n} \{ j(u) + (1 - ku)u'p' - (c^2 \nabla u + b \nabla u') \cdot \nabla p \\
+ \frac{\partial}{\partial \nu}((c^2 g + bg')p) + (c^2 g + bg' \kappa)p \} h \cdot \nu d\sigma.
\]

(60)

Above \( u \) and \( p \) denote the solution of the Westervelt equation (5), respectively the adjoint equation (55) and \( \kappa \) stands for the mean curvature of \( \Gamma_n \).

Proof. Let \( \Omega_t \) be a perturbation of the reference domain \( \Omega \) and \( u_t \) be the solution of the Westervelt equation defined on \( \Omega_t \) as discussed in Section 3. The cost related to the perturbed domain is in view of Lemma 3 given by

\[
J(\Omega_t) = \int_0^T \int_{\Omega} (u_t - y_t)^2 \delta_t dx d\sigma
\]

Mimicking the rearrangement technique in [9] we write the difference of the cost of the perturbed and nominal domain in the following way

\[
J(\Omega_t) - J(\Omega) = \int_0^T \int_{\Omega} ((\delta_t - 1)(u_t - y_t)^2 + (u_t - u)^2 - 2(u_t - u)(y_t - y_d) + (y_t - y_d)^2 + 2(u_t - u)(u - y_d) - 2(u - y_d)(y_t - y_d)) dx d\sigma.
\]

Since \( t \mapsto y_t \) is differentiable at \( t = 0 \), using Theorem 5, we also obtain

\[
\lim_{t \to 0} \frac{1}{t} \int_0^T \int_{\Omega} (u_t - u)^2 dx d\sigma = 0,
\]

\[
\lim_{t \to 0} \frac{1}{t} \int_0^T \int_{\Omega} (u_t - u)(y_t - y_d) dx d\sigma = 0,
\]

\[
\lim_{t \to 0} \frac{1}{t} \int_0^T \int_{\Omega} (y_t - y_d)^2 dx d\sigma = 0.
\]

This together with (47), Lemma 4 and Theorem 5 yields

\[
dJ(\Omega)h = \lim_{t \to 0} \frac{1}{t} (J(\Omega_t) - J(\Omega)) = \int_0^T \int_{\Omega} \left( j(u) \text{div} h - dj(u) \nabla y_d \cdot h \right) dx d\sigma + \lim_{t \to 0} \frac{1}{t} \int_0^T (dj(u), u^t - u) d\sigma.
\]

(61)

The last term can be replaced by means of (59) with \( \phi = u^t - u \). In order to handle the first term in (59) we note the identity

\[
(1 - 2ku)(u^t - u) = k(u^t - u)^2 + (1 - ku)u^t - (1 - ku)u,
\]

which integrating by parts in time leads to

\[
\int_0^T (dj(u), u^t - u) d\sigma = k \int_0^T ((u^t - u)^2, p'') d\sigma
\]
This together with the limits given in Lemma 4 which hold uniformly in \( x \) result in

\[
\lim_{t \to 0} \frac{1}{t} \int_0^T (u_t^t - u) \, d\sigma = \int_0^T ( (1-ku')p'' + b \nabla (u - u')) \, d\sigma
\]

\[
= - \int_0^T (\nabla ((1-ku')p''), h) \, d\sigma + \int_0^T \int_{\Gamma_n} ((1-ku')p'' \cdot h) \, d\gamma \, d\sigma
\]

\[
= \int_0^T ((1-2ku)''p', \nabla u) \, d\sigma + \int_0^T ((1-ku)u'') \cdot \nabla \cdot h \, d\sigma
\]

Above we have rearranged the terms in such a way that the last two lines can be replaced by (58) with \( t \neq 0 \) and \( t = 0 \) respectively. In view of the estimate

\[
| \int_0^T (u_t^t - u)^2 \, d\sigma | \leq C_{\Omega, A}^2 \sqrt{T} \| u_t^t - u \|_{L^2(\Omega)} \| p'' \|_{L^2(\mathcal{L}^2)}
\]

we infer by Theorem 5

\[
\lim_{t \to 0} \frac{1}{t} \int_0^T (u_t^t - u)^2 \, d\sigma = 0.
\]

This together with the limits given in Lemma 4 which hold uniformly in \( x \) result in

\[
\lim_{t \to 0} \frac{1}{t} \int_0^T (dj(u), u_t^t - u) \, d\sigma
\]

\[
= \int_0^T \left( (1-ku')p' + b \nabla (u - u') \right) \, d\sigma
\]

\[
+ \lim_{t \to 0} \frac{1}{t} \left\{ \int_0^T \int_{\Gamma_n} (c^2 g^t + b(g^t)^2)p \, d\gamma \, d\sigma - \int_0^T \int_{\Gamma_n} (c^2 g + b g')p \, d\gamma \, d\sigma \right\}
\]

\[
= I + II + III
\]

(62)

In the first term integration by parts with respect space and time (note that \( h \) does not depend on time) gives rise to

\[
I = - \int_0^T (\nabla ((1-ku')p''), h) \, d\sigma + \int_0^T \int_{\Gamma_n} ((1-ku')p'' \cdot h) \cdot \nu \, d\gamma \, d\sigma
\]

\[
= \int_0^T ((1-2ku)''p', \nabla \cdot h) \, d\sigma + \int_0^T ((1-ku)u'') \cdot \nabla \cdot h \, d\sigma
\]
The last equality follows from the fact that
\[ \partial_p \]

The second term of (62) is dealt with Lemma 6 which gives rise to
\[ II = \int_0^T (c^2 \Delta u + b \Delta u', h \cdot \nabla p) + (c^2 \Delta p - b \Delta p', h \cdot \nabla u)) \, ds \]
\[ + \int_0^T \left\{ \int_{\Gamma_n} (c^2 \nabla u + b \nabla u') \cdot \frac{\partial p}{\partial n} \, d\gamma + \int_{\Gamma_n} \frac{\partial}{\partial n} (c^2 u + b u') h \cdot \nabla p \, d\gamma \right\} \, ds \]
\[ - \int_0^T \int_{\Gamma_n} (c^2 \nabla u + b \nabla u') \cdot \nabla p \, d\gamma \, d\sigma \]
\[ = - \int_0^T (c^2 \Delta u + b \Delta u', h \cdot \nabla p) + (c^2 \Delta p - b \Delta p', h \cdot \nabla u)) \, ds \]
\[ + \int_{\Gamma_n} \frac{\partial}{\partial n} (c^2 u + b u') h \cdot \nabla p \, d\gamma \, d\sigma \]
\[ - \int_0^T \int_{\Gamma_n} (c^2 \nabla u + b \nabla u') \cdot \nabla p \, h \cdot \nu \, d\gamma \, d\sigma. \]

The last equality follows from the fact that \( \frac{\partial p}{\partial n} \) vanishes identically on \( \Gamma_n \). In the last term of (62) we use Lemma 3 as follows

\[ III = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^T \int_{\Gamma_n} (c^2 g' + b(g')') \omega \nu \, d\gamma \, d\sigma - \int_0^T \int_{\Gamma_n} (c^2 g + b g') p \, d\gamma \, d\sigma \]
\[ = \frac{d}{dt} \int_0^T \int_{\Gamma_n} (c^2 g + b g') p \circ F^{-1} \, d\gamma \, d\sigma \big|_{t=0} \]
\[ = \frac{d}{dt} \int_0^T \int_{\Gamma_n} (c^2 g + b g')(p \circ F^{-1}) \, d\gamma \, d\sigma \big|_{t=0} \]
\[ = \int_0^T \int_{\Gamma_n} (c^2 g + b g') (-\nabla p \cdot h) \, d\gamma \]
\[ + \int_{\Gamma_n} \left( \frac{\partial}{\partial n} (c^2 g + b g')p \right) h \cdot \nu \, d\gamma \right\} \, ds. \]

Finally we insert the above expressions into (61)
\[ dJ(\Omega)h = \int_0^T \int_\Omega j(u) \text{div} h \, dx \, ds - \int_0^T \int_\Omega d_j(u) \nabla y_d \cdot h \, dx \, ds \]
\[ + \int_0^T \left\{ \left( (1 - 2ku)p'' - c^2 \Delta u + b \Delta u', \nabla u \cdot h \right) \right\} \, ds \]
\[ + \int_0^T \left\{ \left( (1 - ku)u'' - c^2 \Delta u - b \Delta u', \nabla p \cdot h \right) \right\} \, ds \]
\[ + \int_0^T \int_{\Gamma_n} \left( \frac{\partial}{\partial n} (c^2 u + b u') - (c^2 g + b g')h \cdot \nabla p \right) \, d\gamma \, d\sigma \]
\[ + \int_0^T \int_{\Gamma_n} \left\{ \left( (1 - ku)u'p' - (c^2 \nabla u + b \nabla u', \nabla p) \right) \right\} \, d\gamma \, d\sigma \]
\[ + \frac{\partial}{\partial n} (c^2 g + b g')p \right) + (c^2 g + b g')p \kappa \right\} h \cdot \nu \, d\gamma \, d\sigma. \]

The expressions in the third and fourth line above vanish because of (5), in the second line one can use the strong form of the adjoint equation (55) which results
in
\[
dJ(\Omega)h
= \int_0^T \int_{\Omega} j(u) \text{div} \, h \, dx \, ds - \int_0^T \int_{\Omega} dj(u) \nabla y_d \cdot h \, dx \, ds + \int_0^T (dj(u), \nabla u \cdot h) \, ds
+ \int_0^T \int_{\Gamma} \{ ((1 - ku)u)'p' - (c^2\nabla u + b\nabla u)', \nabla p) \\
+ \frac{\partial}{\partial \nu}((c^2g + bq')p + (c^2g + bq')p\kappa) \} \, h \cdot \nu \, d\gamma \, ds.
\]

The first three terms can be simplified as follows
\[
\int_0^T \int_{\Omega} j(u) \text{div} \, h \, dx \, ds - \int_0^T \int_{\Omega} dj(u) \nabla y_d \cdot h \, dx \, ds + \int_0^T (dj(u), \nabla u \cdot h) \, ds
= \int_0^T \int_{\Omega} j(u) \text{div} \, h \, dx \, ds + \int_0^T \int_{\Omega} dj(u) \nabla (u - y_d) \cdot h \, dx \, ds
= \int_0^T \int_{\Omega} \text{div} (j(u)h) \, dx \, ds = \int_0^T \int_{\Gamma} j(u)h \cdot \nu \, d\gamma \, ds.
\]

Inserting the last expression into \(dJ(\Omega)h\) completes the proof of the existence of the Eulerian derivative of \(J\). By the representation of \(dJ(\Omega)h\) it is obvious that \(dJ(\Omega) \in D^*\) holds.

5. Conclusions and remarks. In this paper, we have rigorously computed the shape derivative for the problem of designing the excitation boundary part in high intensity focused ultrasound lithotripsy, relying on the variational framework from [9]. For this purpose, we have proven regularity results for solutions of the underlying model, i.e., the Westervelt equation with absorbing and inhomogeneous Neumann boundary conditions.

Future work will be concerned with the development and implementation of an numerical optimization algorithm based on the shape sensitivity results from this paper.

Appendix. To see \(H^s(\partial \Omega)\) regularity of a piecewise \(H^s\) function with \(s \in (0, \frac{1}{2})\), it suffices to consider the case of a piecewise \(H^s\) function on a flat domain, since \(H^s(\partial \Omega)\) is defined via local \(C^1\) transformations of the boundary on subsets of \(\mathbb{R}^2\). (The result is actually independent of the space dimension.)

So let \(D \subseteq \mathbb{R}^2\) be composed of a bounded open Lipschitz subdomain \(D_a\) and its complement, i.e., \(D = D_a \cup D_n, D_a \cap D_n = \emptyset\) and consider a piecewise defined function
\[
q = \begin{cases} 
q_a \text{ on } D_a \\
q_n \text{ on } D_n
\end{cases}
\]
with \(q_a = q|_{D_a} \in H^s(D_a), q_n = q|_{D_n} \in H^s_0(D_n)\). We prove that \(q \in H^s(D)\) and
\[
\|q\|_{H^s(D)} \leq \|q_a\|_{H^s(D_a)} + \|q_n\|_{H^s(D_n)}.
\]

For this purpose, we will write \(q = q^a + q^n\) with
\[
q^a = \begin{cases} 
q_a \text{ on } D_a \\
0 \text{ on } D_n
\end{cases}, \quad q^n = \begin{cases} 
0 \text{ on } D_a \\
q_n \text{ on } D_n
\end{cases}
\]
and prove \( q^a \in H^s(D) \) with \( \|q^a\|_{H^s(D)} \leq \|q_n\|_{H^s(D_n)} \), and likewise for \( q^n, q_n \), which by the triangle inequality will yield the assertion. Fix \( \epsilon > 0 \). By \([8, \text{Corollary 1.4.4.5.}]\), which states that \( H^s_0(D_n) = H^s(D_n) \) for \( s \in (0, \frac{1}{2}) \) and \( D_n \) an open Lipschitz domain, there exists a sequence \( (q_{a,k})_{k \in \mathbb{N}} \subseteq C_0^\infty(D) \) such that
\[
\|q_{a,k} - q_n\|_{H^s(D_n)} \to 0 \quad \text{as} \quad k \to \infty.
\]
(63)
For \( (q^a_k)_{k \in \mathbb{N}} \) defined by
\[
q^a_k = \begin{cases} 
q_{a,k} \text{ on } D_n \\
0 \text{ on } D_n \nend{cases}
\]
we have \( \|q^a_k\|_{H^s(D)} = \|q_{a,k}\|_{H^s(D_n)} \leq \|q_a\|_{H^s(D_n)} + \epsilon \) for \( k \) sufficiently large, hence there exists a subsequence, again denoted by \( (q^a_k)_{k \in \mathbb{N}} \), and an element \( q^a \in H^s(D) \) such that
\[
q^a_k \xrightarrow{H^s} q^a\text{ and } q^a_k \xrightarrow{L^2} q^a.
\]
(64)
For any \( \chi \in C_0^\infty(D) \) with support contained in \( D_n \) we have
\[
(q^a_k - q^a, \chi)_{L^2(D)} = \lim_{k \to \infty} (q^a_k, \chi)_{L^2(D_n)} - (q_a, \chi|_{D_n})_{L^2(D_n)} = \lim_{k \to \infty} (q_{a,k} - q_a, \chi|_{D_n})_{L^2(D_n)} = 0
\]
and for any \( \chi \in C_0^\infty(D) \) with support contained in \( D_n \) we have
\[
(q^a_k - q^a, \chi)_{L^2(D)} = \lim_{k \to \infty} (q^a_k, \chi)_{L^2(D_n)} - 0 = 0.
\]
Since \( \{\chi \in C_0^\infty(D) : \text{supp}(\chi) \subseteq D_n\} + \{\chi \in C_0^\infty(D) : \text{supp}(\chi) \subseteq D_n\} \) is dense in \( L^2(D) \), this implies \( q^a = q^a \). As \( \epsilon > 0 \) was arbitrary, this proves the assertion. The proof is the same for \( q^n \), with the only difference that due to the assumption \( q_n \in H^s_0(D_n) \), we need not (and cannot, since \( D_n \) in general cannot be open as well) employ \([8, \text{Corollary 1.4.4.5.}]\).

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