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Sensitivity analysis of linear and nonlinear lithotripter models†

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In this paper, we perform a sensitivity analysis for shape optimization problems arising in models we suggest for a lithotripter. More precisely, we use two models based on high intensity ultrasound focusing by an acoustic lens, where through changing the shape of the lens we try to achieve a favourable focusing. The models are based on acoustic wave equations with piecewise constant coefficients, a linear and a nonlinear one, where for the nonlinear one we use the Westervelt equation. The sensitivity analysis is performed using an adjoint approach.

1 Introduction

The motivation for this work comes from medical application of ultrasound in the non-invasive treatment of kidney stones by the Extracorporreal Shock Wave Lithotripsy. A lithotripter, which is the medical device used for this purpose, attempts to break up the stone with minimal collateral damage by using an externally applied, focused, high-intensity acoustic pulse, see Figure 1.

We want to make a model that describes this procedure. The goal is to minimize the side effects, meaning the effects of ultrasound on the healthy tissue.

The main part of a lithotripter is depicted in Figure 2 as well as the principle according to which it works. It consists of a cylinder filled with fluid (water) in which an acoustic lens is immersed. The excitation comes from an electromagnetic source at the bottom of the cylinder, propagates through the fluid and the focusing is achieved by the silicone lens.

One should note that in our model due to the very similar material properties, we do not make a distinction between the fluid in the lithotripter and the tissue of the patient, i.e. we have only two different parts of the domain in question, the lens and the fluid.

To describe the domain mathematically, we use the fact that it is rotationally symmetric. To describe the lens, we use two functions for the upper and for the lower surfaces with the same value at the right-hand end. We also use the coordinates of the corner point of

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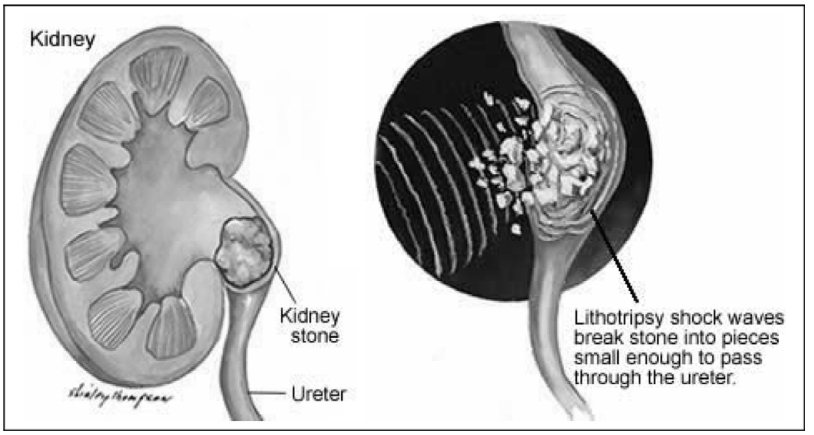


FIGURE 1. Kidney stone and lithotripsy.

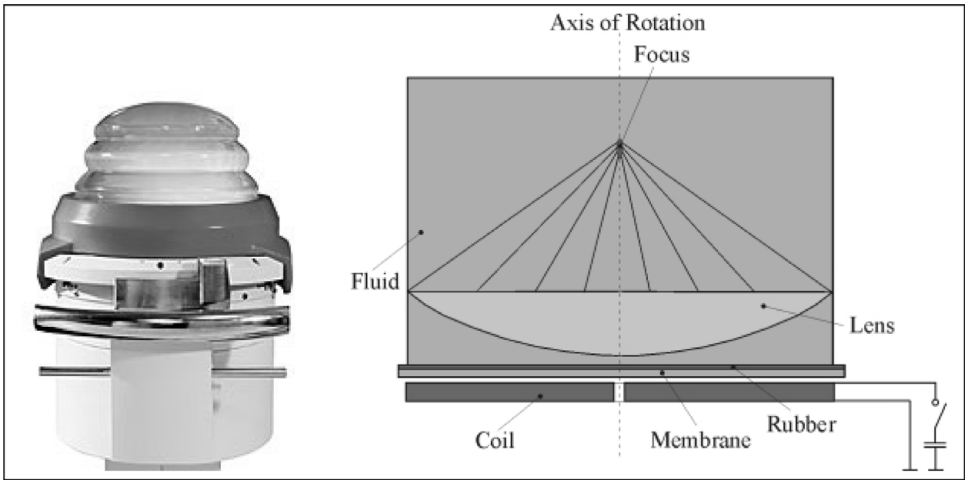


FIGURE 2. Dornier lithotripter and its principle.

the lens as parameters. With this idea, we define

$$\Omega = \left\{(x_1, x_2, x_3) \in \mathbb{R}^3 | x_1^2 + x_2^2 \leqslant R,\ 0 \leqslant x_3 \leqslant H_{\max}\right\}, \tag{1.1}$$

where R and $H_{\max}$ are given constants. Subdomains are defined as

$$\Omega_s = \left\{ x \in \Omega | H + q^l\left(\sqrt{\frac{x_1^2 + x_2^2}{L^2}}\right) < x_3 < H + q^u\left(\sqrt{\frac{x_1^2 + x_2^2}{L^2}}\right)\right\}, \tag{1.2}$$

$$\Omega_f = \Omega \setminus \Omega_s, \tag{1.3}$$

and

$$\Omega_J = \{x \in \Omega_f | x_3 \geqslant H_{\min} > H\}, \tag{1.4}$$

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where

$$C^1_{\diamond}(0,1) = \{\varphi \in C^1[0,1] | \varphi(1) = 0\},$$

and $q^l, q^u \in C^1_{\diamond}(0,1)$.

In the definition above, Ω_s represents the acoustic lens, Ω_f the fluid and Ω_J the human tissue, with (L,H) being the coordinate of the corner point of the lens. We point out again that $\Omega_J \subset \Omega_f$. Furthermore, we assume that the propagation speed of ultrasound is different and constant inside each of Ω_s and Ω_f. Due to rotational symmetry of the domain, we can restrict ourselves to any halfplane that contains the axis of symmetry.

We will consider two lithotripter models, a linear and a nonlinear one. In the first model the ultrasound propagation is described by means of linear acoustic wave equation. The second model makes use of the Westervelt equation of nonlinear acoustics for the same purpose. In the both cases we assume that the material density is constant in the entire domain. In contrast to the linear model, by using the Westervelt equation, we are able to describe nonlinear effects and dissipation. The Westervelt equation can be seen as a simplification – in the situation of local effects being dominated by cumulative effects – of the Kuznetsov equation, which, in turn, is a second-order approximation for viscous heat-conducting fluids of the following equation (cf. [15])

$$-D_t^2\phi + c^2\Delta\phi = \left(D_t + \frac{1}{2}\nabla\phi\cdot\nabla\right)(\nabla\phi)^2 \tag{1.5}$$

for the acoustic velocity potential ϕ. The previous equation describes nonlinear wave propagation in lossy and compressible fluid media.

2 Linear model for a lithotripter

2.1 PDE

The initial-boundary value problem which will be used to describe ultrasound propagation in the domain is given by

$$\begin{aligned}
\frac{1}{c^2}D_t^2 u - \Delta u &= 0 \quad && \text{in } (0,T)\times\Omega,\\
\frac{\partial u}{\partial \nu} &= g \quad && \text{on } (0,T)\times\Gamma_0,\\
D_t u + c\frac{\partial u}{\partial \nu} &= 0 \quad && \text{on } (0,T)\times\hat{\Gamma},\\
\frac{\partial u}{\partial \nu} &= 0 \quad && \text{on } (0,T)\times(\partial\Omega\setminus(\Gamma_0\cup\hat{\Gamma})),\\
u(0,\cdot) = D_t u(0,\cdot) &= 0 \quad && \text{in } \Omega,
\end{aligned} \tag{2.1}$$

where we assume that Ω is C^1 smooth (so that all trace and embedding theorems used here apply), and $\hat{\Gamma} \subset \partial\Omega \setminus \Gamma_0$. Here u plays the role of the acoustic pressure (see the definition of the cost function below.) The excitation is done via the Neumann boundary condition g on $\Gamma_0 \subset \partial\Omega$, which can be prescribed via the normal acceleration of the membrane of the electromagnetic source.

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So we are using one equation in the entire domain, having the speed of sound piecewise constant in different subdomains

$$c(x) = \begin{cases} c_s & x \in \Omega_s \\ c_f & x \in \Omega_f, \end{cases} \tag{2.2}$$

with $\underline{c} \leqslant c_s, c_f \leqslant \overline{c}$.

For the sensitivity analysis we will be using the weak formulation of the PDE (2.1)

$$\int_\Omega \frac{1}{c^2} D_t^2 uw \, dx + \int_\Omega \nabla u \nabla w \, dx + \frac{1}{c} \int_{\hat{\Gamma}} D_t uw \, d\Gamma = \int_{\Gamma_0} gw \, d\Gamma, \quad \forall w \in H^1(\Omega). \tag{2.3}$$

Remark 2.1.1 *The formulation of the problem (2.1) should be understood in context of domain decomposition. It is implicitly assumed that u is continuous across the interface along with normal derivative. Also, it is assumed that the material density in the entire domain is constant, so that this form of acoustic wave equation can be used. A well-posedness analysis for the problem (2.1) can be found in [2] for the case of absorbing boundary conditions on the whole boundary, which carries over to our situation of mixed boundary conditions in a straightforward manner, see also [10], Theorems 3 and 5 in Section 7.2.2. It yields existence of a weak solution $u \in W(0,T)$ of (2.3), where*

$$W(0,T) = \left\{ u \in L^\infty(0,T;H^1(\Omega)) \,|\, D_t u \in L^\infty(0,T;L^2(\Omega)) \right\} \subset H^1((0,T) \times \Omega).$$

2.2 Regularity of u

Proposition 1 *Let $c \in L^\infty(\Omega)$ with $\underline{c} \leqslant c(x) \leqslant \overline{c}$, let*

$$g \in W^{m+1,1}(0,T;H^{-1/2}(\partial\Omega)) \cap W^{m,\infty}(0,T;H^{-1/2}(\partial\Omega))$$

for some $m \in \mathbf{N}_0$ and let the compatibility condition

$$(D_t^k g)(0,\cdot) = 0 \text{ on } \partial\Omega \text{ for all } k \leqslant m$$

hold. Then the weak solution $u \in W(0,T)$ of (2.3) lies in $W^{m+1,\infty}(0,T;L^2(\Omega)) \cap W^{m,\infty}(0,T;H^1(\Omega))$ and if $m \geqslant 2$, additionally $\Delta u \in W^{m-2,\infty}(0,T;H^1(\Omega))$.

Proof Let us consider $(g_n)_{n\in\mathbf{N}} \subset C_0^\infty(\Omega)$, $(c_n)_{n\in\mathbf{N}} \subset C^\infty(\Omega)$ with $c_n^2 \to c^2$ in $L^p(\Omega)$ for some $p \geqslant 3$, $\underline{c} \leqslant c_n(x) \leqslant \overline{c}$, $g_n \to g$ in $W^{m+1,1}(0,T;H^{-1/2}(\partial\Omega)) \cap W^{m,\infty}(0,T;H^{-1/2}(\partial\Omega))$ and let u_n be the (classical) solution of (2.1) with c_n, g_n in place of c, g, which is smooth by the usual regularity results for the wave equation, see, e.g. [10].

Since c_n is independent of t, $U_n^m := D_t^m u_n$ solves (2.1) with g replaced by $D_t^m g$. Hence, by multiplying the PDE in (2.1) with $D_t U_n^m$, integrating by parts with respect to space,

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and integrating over $(0,t)$ we get (as usual) the energy estimate

$$\begin{aligned}
&\max\left\{\frac{1}{\bar{c}^2}\,\|D_tU_n^m\|^2_{L^\infty(0,T;L^2(\Omega))},\,\|\nabla U_n^m\|^2_{L^\infty(0,T;L^2(\Omega))}\right\}\\
&\quad\leqslant 2\sup_t\Big|\int_0^t\int_{\Gamma_0} D_t^m g_n D_tU_n^m\,d\Gamma\,d\tau\Big|\\
&\quad= 2\sup_t\Big|-\int_0^t\int_{\Gamma_0} D_t^{m+1}g_nU_n^m\,d\Gamma\,d\tau+\int_{\Gamma_0} D_t^m g_n(t)U_n^m(t)\,d\Gamma\Big|\\
&\quad\leqslant 2C_1\left\|D_t^{m+1}g_n\right\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}\|U_n^m\|_{L^\infty(0,T;H^1(\Omega))}\\
&\qquad+2C_1\|D_t^m g_n\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\|U_n^m\|_{L^\infty(0,T;H^1(\Omega))}\\
&\quad\leqslant 2C_1^2\big(\left\|D_t^{m+1}g_n\right\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}+\|D_t^m g_n\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\big)^2\\
&\qquad+\frac{1}{2}\,\|U_n^m\|^2_{L^\infty(0,T;H^1(\Omega))},
\end{aligned}$$

where C_1 is the constant in the trace theorem $\gamma : H^1(\Omega)\to H^{1/2}(\partial\Omega)$, so that using $D_tU_n^m = U_n^{m+1}$ we end up with

$$\begin{aligned}
&\max\left\{\frac{1}{\bar{c}^2}\left\|U_n^{m+1}\right\|^2_{L^\infty(0,T;L^2(\Omega))},\frac{1}{2}\,\|\nabla U_n^m\|^2_{L^\infty(0,T;L^2(\Omega))}\right\}\\
&\quad\leqslant\frac{1}{2}\,\|U_n^m\|^2_{L^\infty(0,T;L^2(\Omega))}\\
&\qquad+2C_1^2\left(\left\|D_t^{m+1}g_n\right\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}+\|D_t^m g_n\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\right)^2,
\end{aligned}$$

which inductively yields a bound depending only on $\bar{c}$, C_1 and $\|g_n\|_{W^{m+1,1}(0,T;H^{-1/2}(\partial\Omega))\cap W^{m,\infty}(0,T;H^{-1/2}(\partial\Omega))}$ (but not on c_n!) for

$$\left\|U_n^{m+1}\right\|^2_{L^\infty(0,T;L^2(\Omega))}\ \text{and}\ \|\nabla U_n^m\|^2_{L^\infty(0,T;L^2(\Omega))}.$$

The difference $u-U_n^0$ satisfies

$$\begin{aligned}
\frac{1}{c^2}D_t^2(u-U_n^0)-\Delta(u-U_n^0)&=\left(\frac{1}{c_n^2}-\frac{1}{c^2}\right)D_t^2U_n^0 \quad \text{in } (0,T)\times\Omega\\
\frac{\partial(u-U_n^0)}{\partial\nu}&=g-g_n \quad \text{on } (0,T)\times\Gamma_0\\
D_t(u-U_n^0)+c\frac{\partial(u-U_n^0)}{\partial\nu}&=0 \quad \text{on } (0,T)\times\hat{\Gamma}\\
\frac{\partial(u-U_n^0)}{\partial\nu}&=0 \quad \text{on } (0,T)\times(\partial\Omega\setminus(\Gamma_0\cup\hat{\Gamma}))\\
(u-U_n^0)(0,\cdot)=D_t(u-U_n^0)(0,\cdot)&=0 \quad \text{in } \Omega
\end{aligned}\tag{2.4}$$

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so by the same procedure as above we arrive at

$$\begin{aligned}
&\max\left\{\frac{1}{\bar{c}^2}\left\|D_t(u-U_n^0)\right\|^2_{L^\infty(0,T;L^2(\Omega))}, \left\|\nabla(u-U_n^0)\right\|^2_{L^\infty(0,T;L^2(\Omega))}\right\}\\
&\quad\leqslant 2\sup_t\left(\left|\int_0^t\int_\Omega\left(\frac{1}{c_n^2}-\frac{1}{c^2}\right)D_t^2U_n^0D_t(u-U_n^0)\,dx\,dt\right|\right.\\
&\qquad\left.+\left|-\int_0^t\int_{\Gamma_0}D_t(g-g_n)(u-U_n^0)\,d\Gamma\,d\tau+\int_{\Gamma_0}(g-g_n)(t)(u-U_n^0)(t)\,d\Gamma\right|\right)\\
&\quad\leqslant 2\left\|\frac{1}{c_n^2}-\frac{1}{c^2}\right\|_{L^p(\Omega)}\left\|U_n^2\right\|_{L^2(0,T;L^{\frac{2p}{p-2}}(\Omega))}\left\|D_t(u-U_n^0)\right\|_{L^2(0,T;L^2(\Omega))}\\
&\qquad+2C_1\Big(\|D_t(g-g_n)\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}+\|g-g_n\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\Big)\\
&\qquad\left\|u-U_n^0\right\|_{L^\infty(0,T;H^1(\Omega))},
\end{aligned}$$

where we have used Hölder's inequality. Hence using the estimate

$$\|v\|_{L^\infty(0,T;L^2(\Omega))}\leqslant 2T\,\|D_tv\|_{L^\infty(0,T;L^2(\Omega))},\tag{2.5}$$

if $v(0)=0$, following from the identity

$$\|v(t)\|^2_{L^2(\Omega)}=\|v(0)\|^2_{L^2(\Omega)}+2\int_0^t\langle D_tv(\sigma),v(\sigma)\rangle_{L^2(\Omega)}\,d\sigma,$$

for $v=u-U_n^0$, we arrive at

$$\begin{aligned}
&\max\left\{\left\|D_t(u-U_n^0)\right\|_{L^\infty(0,T;L^2(\Omega))},\left\|u-U_n^0\right\|_{L^\infty(0,T;H^1(\Omega))}\right\}\\
&\quad\leqslant C_3\Big(\sqrt{\left\|\frac{1}{c_n}-\frac{1}{c^2}\right\|_{L^p(\Omega)}\left\|U_n^2\right\|_{L^2(0,T;L^{\frac{2p}{p-2}}(\Omega))}}\\
&\qquad+\|D_t(g-g_n)\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}+\|g-g_n\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\Big),
\end{aligned}\tag{2.6}$$

with some constant C_3 depending only on C_1 and $\bar{c}$, and the right-hand side goes to zero as $n\to\infty$, since by $p\geqslant 3$ we have $\frac{2p}{p-2}\leqslant 6$, so that $H^1(\Omega)$ is continuously embedded in $L^{\frac{2p}{p-2}}(\Omega)$. Thus, we can conclude that U_n^0 converges to u in the topology given by the norms on the left-hand side of (2.6). Analogously we get convergence of U_n^m to D_t^mu, since due to the independence of $\frac{1}{c_n^2}-\frac{1}{c^2}$ of t, differentiation of (2.4) with respect to t only affects U_n^2 (which becomes U_n^{m+2}) in the right-hand side of (2.6).

To show additional regularity if $m\geqslant 2$ namely uniform boundedness of the gradient of u, observe that we can further conclude $D_t^mu\in L^\infty(0,T;H^1(\Omega))\subset L^\infty(0,T;L^6(\Omega))$, hence multiplication with the $L^\infty(\Omega)$ coefficient $\frac{1}{c^2}$ still gives an $L^\infty(0,T;L^6(\Omega))$ function, which by the PDE translates to $\Delta D_t^{m-2}u$

$$\Delta D_t^{m-2}u=\frac{1}{c^2}D_t^mu\in L^\infty(0,T;L^6(\Omega)),$$

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from which we conclude

$$\nabla D_t^{m-2} u \in L^\infty(0,T;W^{1,6}(\Omega)) \subset L^\infty(0,T;C^{0,\gamma}(\Omega)), \tag{2.7}$$

for all $\gamma \in (0, \frac{1}{2})$. □

2.3 Optimization problem

In order to formulate the optimization problem we want to solve, a cost functional has to be defined first. We do it in the following way

$$j(\alpha) = J(u(\alpha)) = \int_0^T \int_{\Omega_J} |u - u^d|^2 \, dx \, dt, \tag{2.8}$$

where $u = u(\alpha)$ solves (2.1). This means that we have a prescribed pressure distribution u^d with a peak in the desired focus and close to zero elsewhere. Ω_J is a fixed (independently of the lens shape) subset of the fluid region, since penalization of deviations from the desired pressure distribution should mainly take place within the human tissue.

As we pointed out earlier, the functions q^l, q^u as well as the corner point given by the coordinates (L, H) serve as design variables. So, we define the space of admissible designs as

$$\begin{aligned} U^{ad} = \{&\alpha \in C^1([0,1], \mathbb{R}^2) \times \mathbb{R}^2 | \alpha_{\min} \leqslant \alpha^i \leqslant \alpha_{\max}, \\ &\alpha^i(1) = 0, \quad |\alpha^{i\prime}| \leqslant M \text{ a.e.}, i \in \{1,2\}\}, \end{aligned}$$

with $\alpha = (q^u, q^l, H, L)$.

Now, the optimization problem reads as follows:

$$\begin{cases} \text{Find } \alpha^* \in U^{ad} \text{ such that} \\ J(u(\alpha^*)) \leqslant J(u(\alpha)) \qquad \forall \alpha \in U^{ad}, \end{cases} \tag{2.9}$$

where u solves

$$\begin{cases} \text{Find } u = u(\alpha) \in W(0,T) \\ \text{such that (2.3) holds with } c = c_\alpha. \end{cases} \tag{2.10}$$

In order to prove existence of a solution to the optimization problem, we are going to use the abstract setting of optimal shape design problems developed in section 2.4 of [9].

For well-posedness and regularity of a solution to (2.10) we refer to Remark 2.1.1 and Proposition 1.

According to theorem 2.10 in [9], existence of solutions to (2.9) will follow after verifying assumptions $(\mathscr{B}_1)$ and $(\mathscr{B}_2)$ introduced in section 2.4 of [9]. We provide these assumptions and the theorem in the Appendix (see Theorem A.0.2).

Lemma 1 (Verification of $(\mathscr{B}_1)$) *Let $g \in W^{1,1}(0,T;H^{-1/2}(\partial\Omega)) \cap L^\infty(0,T;H^{-1/2}(\partial\Omega))$. For any sequence $\{(\alpha_n, u_n)\}$, where $\alpha_n \in U^{ad}$ and $u_n := u(\alpha_n) \in H^1((0,T) \times \Omega)$ is a solution of (2.10), there exists a subsequence, denoted again by $\{(\alpha_n, u_n)\}$, and elements $\alpha \in U^{ad}$, $u \in$*

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$H^1((0,T)\times\Omega)$ *such that*

$$\left.\begin{array}{l}\alpha_n \to \alpha \text{ in } C([0,1],\mathbb{R}^2)\times\mathbb{R}^2\\ u_n \rightharpoonup u \text{ in } H^1((0,T)\times\Omega),\end{array}\right\} \qquad n\to\infty.$$

In addition, u solves (2.10).

Proof Since set U^{ad} is pointwise bounded and equicontinuous, by the Arzelà-Ascoli theorem U^{ad} is also uniformly bounded and for each sequence $\{\alpha_n\}\in U^{ad}$ there exists a subsequence which converges uniformly on $[0,1]$. In order to find a subsequence of the sequence $\{u_n\}$ which converges weakly, we establish the $H^1((0,T)\times\Omega)$ boundedness of $\{u_n\}$, with $c_n = c_{\alpha_n}$: Multiplying the PDE for u_n with $D_t u_n$ and integrating with respect to space and time we get, with $\bar c = \max\{c_f, c_s\}$ similarly to the proof of Proposition 1

$$\begin{aligned}&\max\left\{\frac{1}{\bar c^2}\,\|D_t u_n\|^2_{L^\infty(0,T;L^2(\Omega))}, \|\nabla u_n\|^2_{L^\infty(0,T;L^2(\Omega))}\right\}\\ &\quad\leqslant 2\sup_t\Big|\int_0^t\int_{\Gamma_0} g D_t u_n\,d\Gamma\,d\tau\Big|\\ &\quad= 2\sup_t\Big|-\int_0^t\int_{\Gamma_0} D_t g u_n\,d\Gamma\,d\tau+\int_{\Gamma_0} g(t)u_n(t)\,d\Gamma\Big|\\ &\quad\leqslant 2C_1^2\tilde c^2\big(\|D_t g\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}+\|g\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\big)^2+\frac{1}{2\tilde c^2}\,\|u_n\|^2_{L^\infty(0,T;H^1(\Omega))},\end{aligned}$$

for $\tilde c = \max\{2\bar c T, 1\}$, which with (2.5) yields

$$\begin{aligned}&\max\left\{\frac{1}{\bar c^2}\,\|D_t u_n\|^2_{L^\infty(0,T;L^2(\Omega))}, \|\nabla u_n\|^2_{L^\infty(0,T;L^2(\Omega))}\right\}\\ &\quad\leqslant 2C_1^2\tilde c^2\big(\|D_t g\|_{L^1(0,T;H^{-1/2}(\partial\Omega))}+\|g\|_{L^\infty(0,T;H^{-1/2}(\partial\Omega))}\big)^2\\ &\qquad+\frac{1}{2\tilde c^2}\Big(4T^2\,\|D_t u_n\|^2_{L^\infty(0,T;L^2(\Omega))}+\|\nabla u_n\|^2_{L^\infty(0,T;L^2(\Omega))}\Big),\end{aligned}$$

and hence gives us an estimate

$$\|u_n\|_{H^1((0,T)\times\Omega)}\leqslant\sqrt{T}\,\|u_n\|_{W(0,T)}\leqslant C.$$

This implies weak $H^1((0,T)\times\Omega)$ convergence of a subsequence of $\{u_n\}$ to some $u\in H^1((0,T)\times\Omega)$. It remains to prove that u solves (2.10). Let $v\in H^1(\Omega)$ and $\phi\in C_0^\infty(0,T)$ be fixed. Then we have

$$\int_0^T\int_\Omega \frac{1}{c_n^2}D_t^2 u_n v\phi\,dx dt+\int_0^T\int_\Omega \nabla u_n\nabla v\phi\,dx\,dt+\frac{1}{c_f}\int_0^T\int_{\hat\Gamma} D_t u_n v\phi\,d\Gamma\,dt=\int_0^T\int_{\Gamma_0} gv\phi\,d\Gamma\,dt$$

and letting $n\to\infty$ we obtain

$$\int_0^T\int_\Omega \frac{1}{c^2}D_t^2 u v\phi\,dx\,dt+\int_0^T\int_\Omega \nabla u\nabla v\phi\,dx\,dt+\frac{1}{c_f}\int_0^T\int_{\hat\Gamma} D_t u v\phi\,d\Gamma\,dt=\int_0^T\int_{\Gamma_0} gv\phi\,d\Gamma\,dt.$$

In order to justify the previous conclusion we calculate the limit of the first term on the

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left-hand side using the triangle inequality and integrating by parts with respect to time

$$\begin{aligned}
&\left| \int_0^T \int_\Omega \frac{1}{c_n^2} D_t^2 u_n v \phi \, dx \, dt - \int_0^T \int_\Omega \frac{1}{c^2} D_t^2 u v \phi \, dx \, dt \right| \\
&\quad \leqslant \left| \int_0^T \int_\Omega \frac{1}{c^2} (D_t u_n - D_t u) v D_t \phi \, dx \, dt \right| + \left| \int_0^T \int_\Omega \left(\frac{1}{c_n^2} - \frac{1}{c^2} \right) D_t u_n v D_t \phi \, dx \, dt \right| \\
&\quad \leqslant \left| \int_0^T \int_\Omega \frac{1}{c^2} (D_t u_n - D_t u) v D_t \phi \, dx \, dt \right| \\
&\qquad + \left| \left| \frac{1}{c_n^2} - \frac{1}{c^2} \right| \right|_{L^p(\Omega)} ||D_t u_n||_{L^2((0,T)\times\Omega)} ||v D_t \phi||_{L^q((0,T)\times\Omega)} \\
&\quad \to 0,
\end{aligned}$$

with $q = \frac{2p}{p-1}$, since $D_t u_n - D_t u \rightharpoonup 0$ in $L^2((0,T)\times\Omega)$, $c_n \to c$ in $L^p(\Omega)$ for any $p \in [1,\infty)$ by lemma 2.4 in [9] and $||D_t u_n||_{L^2((0,T)\times\Omega)} \leqslant C$. For the second term we have

$$\left| \int_0^T \int_\Omega \nabla u_n \nabla v \phi \, dx \, dt - \int_0^T \int_\Omega \nabla u \nabla v \phi \, dx \, dt \right| = \left| \int_0^T \int_\Omega \nabla (u_n - u) \nabla v \phi \, dx \, dt \right| \overset{n\to\infty}{\longrightarrow} 0,$$

by the weak convergence of u_n in $L^2(0,T;H^1(\Omega))$. A similar argument is applicable also for the third term on the left-hand side. As $v \in H^1(\Omega)$ and $\phi \in C_0^\infty(0,T)$ are arbitrary we conclude that u solves (2.10). □

Lemma 2 (Verification of $(\mathscr{B}_2)$) *The cost functional J is continuous in the following sense:*

$$\left.\begin{aligned} &\alpha_n \to \alpha \text{ in } C([0,1],\mathbb{R}^2) \times \mathbb{R}^2,\ \alpha_n,\ \alpha \in U^{ad} \\ &y_n \rightharpoonup y \text{ in } H^1((0,T)\times\Omega),\ y_n,\ y \in H^1((0,T)\times\Omega) \end{aligned}\right\} \Rightarrow \liminf_{n\to\infty} J(y_n) \geqslant J(y).$$

Proof From $y_n \rightharpoonup y$ in H^1 it follows that the sequence $\{y_n\}$ converges weakly to y also in L^2. Since the norm in any Hilbert space is lower semicontinuous, we obtain

$$y_n \rightharpoonup y \quad \Rightarrow \quad y_n - y^d \rightharpoonup y - y^d \quad \Rightarrow \quad \liminf_{n\to\infty} ||y_n - y^d||_{L^2} \geqslant ||y - y^d||_{L^2}$$

which means $\liminf_{n\to\infty} J(y_n) \geqslant J(y)$. □

Remark 2.3.1 *The proof of Lemma 2 shows that the optimization problem (2.9) remains well-posed if we replace the L^2 norm in the definition of the objective (2.8) by an H^s norm with $s \in (0,1]$.*

2.4 Sensitivity analysis

Here we want to calculate derivatives of the cost functional with respect to the design variables α, but as J depends on α through the solution u to the state equation, we first do the derivation of u with respect to α. Then using the chain rule we calculate the desired derivatives as well. For simplicity of exposition we first of all consider a domain with a

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single interface parametrized by q and fix $H = 0, L = 1$, i.e.

$$\Omega_s = \{x \in \mathbb{R}^3 \mid x_1^2 + x_2^2 \leqslant R, 0 < x_3 < q(\sqrt{x_1^2 + x_2^2})\}$$
$$\Omega_f = \{x \in \mathbb{R}^3 \mid x_1^2 + x_2^2 \leqslant R, q(\sqrt{x_1^2 + x_2^2}) < x_3 < H_{\max}\}$$

and c is defined according to (2.2).

2.4.1 *Derivative of u with respect to q*

For continuity of u w.r.t. q we refer to the proof of Lemma 1.

Forming the difference quotient $\frac{u(q+\epsilon s)-u(q)}{\epsilon}$ in (2.3) and taking the limit $\epsilon \to 0$, we find that $\frac{du}{dq}(q)[s] =: v^s$ solves

$$\begin{aligned}
&\int_\Omega \frac{1}{c^2(q)} D_t^2 v^s w \, dx + \int_\Omega \nabla v^s \nabla w \, dx + \frac{1}{\sqrt{c_f}} \int_{\hat{\Gamma}} D_t v^s w \, d\Gamma \\
&= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_\Omega \left(\frac{1}{c^2(q+\epsilon s)} - \frac{1}{c^2(q)} \right) D_t^2 u(q+\epsilon s) w \, dx \\
&= 2\pi \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_0^1 r \int_{\min\{q(r), q(r)+\epsilon s(r)\}}^{\max\{q(r), q(r)+\epsilon s(r)\}} \left(\frac{1}{c^2(q+\epsilon s)} - \frac{1}{c^2(q)} \right) \overline{\overline{D_t^2 u(q+\epsilon s)}} \overline{\overline{w}} dx_3 dr \\
&= 2\pi \left(\frac{1}{c_f^2} - \frac{1}{c_s^2} \right) \int_0^1 r \overline{\overline{D_t^2 u}}(r, q(r), t) \overline{\overline{w}}(r, q(r)) s(r) \, dr, \qquad (2.11) \\
&\qquad \forall w \in H^1(\Omega), \qquad v^s \in W(0,T)
\end{aligned}$$

where $u = u(q)$ and where we have used continuity of u w.r.t. q and rotational symmetry. Moreover, $\overline{\overline{\phi}}$ denotes the canonical restriction of some rotational symmetric function ϕ to the halfplane given by a cut along the axis of symmetry. By the regularity result Proposition 1, the right-hand side of (2.11) is well defined and in $L^\infty(0,T)$ for all $w \in H^1(\Omega)$, $s \in L^2(0,1)$, provided $g \in W^{3,1}(0,T; H^{-1/2}(\partial\Omega)) \cap W^{2,\infty}(0,T; H^{-1/2}(\partial\Omega))$, by continuity of the trace operator $H^1(\Omega) \to H^{1/2}(\partial\Omega_f \cap \partial\Omega_s) \subseteq L^4(\partial\Omega_f \cap \partial\Omega_s)$, Hölder's inequality, and the fact that the integral on the right-hand side of (2.11) is just the (two-dimensional) surface integral over the interface $\partial\Omega_f \cap \partial\Omega_s$.

2.4.2 *Derivative of j with respect to q*

In order to obtain derivatives of the cost functional we introduce the Lagrangian

$$\begin{aligned}
\mathcal{L}(\xi, \eta; u, w) = J(u) &+ \int_0^T \int_\Omega \frac{1}{c^2} D_t^2 u w \, dx \, dt + \int_0^T \int_\Omega \nabla u \nabla w \, dx \, dt \\
&+ \frac{1}{c_f} \int_0^T \int_{\hat{\Gamma}} D_t u w \, d\Gamma \, dt - \int_0^T \int_{\Gamma_0} g w \, d\Gamma \, dt,
\end{aligned}$$

where $\xi, \eta \in \mathbb{R}$, $u, w \in W(0,T)$, and ξ, η are used to describe a two-parametric family of perturbations

$$q \mapsto q_{\xi\eta} = q + \xi s + \eta h$$

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and $s, h \in C^1_\diamond(0,1)$ are directions of perturbation, as is usual for optimization problems with constraints. We calculate directional derivatives of $\mathscr{L}$ with respect to the third and the fourth argument

$$\begin{aligned}\langle D_u\mathscr{L}(\xi,\eta;u,w);v\rangle &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\mathscr{L}(\xi,\eta;u+\varepsilon v,w)-\mathscr{L}(\xi,\eta;u,w))\\ &= 2\int_0^T\int_{\Omega_J}(u-u^d)v\,dx\,dt+\int_0^T\int_\Omega\frac{1}{c^2}D_t^2vw\,dx\,dt\\ &\quad+\int_0^T\int_\Omega\nabla v\nabla w\,dx\,dt+\frac{1}{c_f}\int_0^T\int_{\hat\Gamma}D_tvw\,d\Gamma\,dt,\end{aligned}\tag{2.12}$$

and

$$\begin{aligned}\langle D_w\mathscr{L}(\xi,\eta;u,w);z\rangle &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\mathscr{L}(\xi,\eta;u,w+\varepsilon z)-\mathscr{L}(\xi,\eta;u,w))\\ &= \int_0^T\int_\Omega\frac{1}{c^2}D_t^2uz\,dx\,dt+\int_0^T\int_\Omega\nabla u\nabla z\,dx\,dt\\ &\quad+\frac{1}{c_f}\int_0^T\int_{\hat\Gamma}D_tuz\,d\Gamma\,dt-\int_0^T\int_{\Gamma_0}gz\,d\Gamma\,dt.\end{aligned}\tag{2.13}$$

In such a way we obtain the two equations

$$\begin{aligned}\langle D_u\mathscr{L}(\xi,\eta;u,w);v\rangle &= 0 \quad \forall v\in W(0,T)\\ \langle D_w\mathscr{L}(\xi,\eta;u,w);z\rangle &= 0 \quad \forall z\in W(0,T)\end{aligned}\tag{2.14}$$

which represent adjoint and state equation, respectively. The strong formulation of the adjoint problem is

$$\begin{aligned}\frac{1}{c^2}D_t^2w-\Delta w &= -2(u-u^d)\chi_{\Omega_J} \quad \text{in } (0,T)\times\Omega\\ D_tw-c\frac{\partial w}{\partial\nu} &= 0 \quad \text{on } (0,T)\times\hat\Gamma\\ \frac{\partial w}{\partial\nu} &= 0 \quad \text{on } (0,T)\times(\partial\Omega\setminus\hat\Gamma)\\ w(T,\cdot)=D_tw(T,\cdot) &= 0 \quad \text{in } \Omega.\end{aligned}\tag{2.15}$$

Having these two equations (2.14) satisfied and denoting their solutions by $u(\xi,\eta)$ and $w(\xi,\eta)$, we have

$$\begin{aligned}\frac{d}{d\xi}\mathscr{L}(\xi,\eta;u(\xi,\eta),w(\xi,\eta)) &= D_\xi\mathscr{L}(\xi,\eta;u,w)+\left\langle D_u\mathscr{L}(\xi,\eta;u,w);\frac{d}{d\xi}u\right\rangle\\ &\quad+\left\langle D_w\mathscr{L}(\xi,\eta;u,w);\frac{d}{d\xi}w\right\rangle\\ &= D_\xi\int_0^T\int_\Omega\frac{1}{c^2}D_t^2uw\,dx\,dt.\end{aligned}$$

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This is due to the fact that explicit dependence of $\mathscr{L}$ on ξ is only through the dependence of $c = c(\xi, \eta)$ on ξ. Hence, we have that

$$\begin{aligned}\frac{d}{d\xi}\mathscr{L}(\xi,\eta;u,w) &= K\int_0^T\int_0^1 r\overline{\overline{D_t^2 u}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\ &= -K\int_0^T\int_0^1 r\overline{\overline{D_t u}}(r,q(r),t)\overline{\overline{D_t w}}(r,q(r),t)s(r)\,dr\,dt \end{aligned} \tag{2.16}$$

in the same way as in (2.11), with the abbreviation $K = 2\pi(\frac{1}{c_f^2} - \frac{1}{c_s^2})$ and integration by parts with respect to time in the last identity. On the other hand, the derivative of the reduced cost $j(\xi,\eta) = J(u(\xi,\eta)) = \mathscr{L}(\xi,\eta;u(\xi,\eta),w(\xi,\eta))$ with respect to ξ is equal to the same derivative of $\mathscr{L}$

$$\frac{d}{d\xi}\mathscr{L}(\xi,\eta;u(\xi,\eta),w(\xi,\eta)) = \frac{\partial j}{\partial \xi}(\xi,\eta). \tag{2.17}$$

Similarly we obtain

$$\frac{\partial j}{\partial \eta} = K\int_0^T\int_0^1 r\overline{\overline{D_t^2 u}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)h(r)\,dr\,dt. \tag{2.18}$$

In order to compute second order derivatives, we look at the preceding situation as in the beginning: we need to find a derivative of $\frac{\partial j}{\partial \xi}$ with respect to η under the constraints imposed by state and adjoint equation. So we introduce the second-order Lagrangian

$$\begin{aligned}\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi) &= \frac{d}{d\xi}\mathscr{L}(\xi,\eta;u,w) + \langle D_u\mathscr{L}(\xi,\eta;u,w);\Psi\rangle + \langle D_w\mathscr{L}(\xi,\eta;u,w);\Lambda\rangle \\ &= K\int_0^T\int_0^1 r\overline{\overline{D_t^2 u}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt + 2\int_0^T\int_{\Omega_J}(u-u^d)\Psi\,dx\,dt \\ &\quad + \int_0^T\int_\Omega \frac{1}{c^2}D_t^2\Psi w\,dx\,dt + \int_0^T\int_\Omega \nabla\Psi\nabla w\,dx\,dt + \frac{1}{c_f}\int_0^T\int_{\hat{\Gamma}} D_t\Psi w\,d\Gamma\,dt \\ &\quad + \int_0^T\int_\Omega \frac{1}{c^2}D_t^2 u\Lambda\,dx\,dt + \int_0^T\int_\Omega \nabla u\nabla\Lambda\,dx\,dt + \frac{1}{c_f}\int_0^T\int_{\hat{\Gamma}} D_t u\Lambda\,d\Gamma\,dt \\ &\quad - \int_0^T\int_{\Gamma_0} g\Lambda\,d\Gamma\,dt. \end{aligned} \tag{2.19}$$

Similarly as before, we find the derivatives of $\mathscr{L}_2$ with respect to its third, fourth, fifth

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and sixth argument

$$\begin{aligned}\langle D_u \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);v\rangle &= K\int_0^T\int_0^1 r\overline{\overline{D_t^2 v}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt\\ &\quad +2\int_0^T\int_{\Omega_J} v\Psi\,dx\,dt+\int_0^T\int_\Omega \frac{1}{c^2}D_t^2 v\Lambda\,dx\,dt+\int_0^T\int_\Omega \nabla v\nabla\Lambda\,dx\,dt\\ &\quad +\frac{1}{c_f}\int_0^T\int_{\hat{\Gamma}} D_t v\Lambda\,d\Gamma\,dt \qquad (2.20)\\ \langle D_w \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);z\rangle &= K\int_0^T\int_0^1 r\overline{\overline{D_t^2 u}}(r,q(r),t)\overline{\overline{z}}(r,q(r),t)s(r)\,dr\,dt\\ &\quad +\int_0^T\int_\Omega \frac{1}{c^2}D_t^2\Psi z\,dx\,dt+\int_0^T\int_\Omega \nabla\Psi\nabla z\,dx\,dt\\ &\quad +\frac{1}{c_f}\int_0^T\int_{\hat{\Gamma}} D_t\Psi z\,d\Gamma\,dt \qquad (2.21)\\ \langle D_\Lambda \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\lambda\rangle &= \int_0^T\int_\Omega \frac{1}{c^2}D_t^2 u\lambda\,dx\,dt+\int_0^T\int_\Omega \nabla u\nabla\lambda\,dx\,dt\\ &\quad +\frac{1}{c_f}\int_0^T\int_{\hat{\Gamma}} D_t u\lambda\,d\Gamma\,dt-\int_0^T\int_{\Gamma_0} g\lambda\,d\Gamma\,dt \qquad (2.22)\\ \langle D_\Psi \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\psi\rangle &= 2\int_0^T\int_{\Omega_J}(u-u^d)\psi\,dx\,dt+\int_0^T\int_\Omega \frac{1}{c^2}D_t^2\psi w\,dx\,dt\\ &\quad +\int_0^T\int_\Omega \nabla\psi\nabla w\,dx\,dt+\frac{1}{c_f}\int_0^T\int_{\hat{\Gamma}} D_t\psi w\,d\Gamma\,dt. \qquad (2.23)\end{aligned}$$

So, the equations to solve in order to calculate the second order derivative of j are

$$\begin{aligned}\langle D_u \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);v\rangle &= 0 \quad \forall v\in W(0,T)\\ \langle D_w \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);z\rangle &= 0 \quad \forall z\in W(0,T)\\ \langle D_\Lambda \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\lambda\rangle &= 0 \quad \forall \lambda\in W(0,T)\\ \langle D_\Psi \mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\psi\rangle &= 0 \quad \forall \psi\in W(0,T)\end{aligned} \qquad (2.24)$$

with solution $(u,w,\Lambda,\Psi)=(u,w,\Lambda,\Psi)(\xi,\eta)$. Now, differentiation with respect to η gives us the second-order derivative of j

$$\begin{aligned}\frac{\partial^2 j}{\partial\xi\partial\eta}(\xi,\eta) &= \frac{d}{d\eta}\mathscr{L}_2(\xi,\eta;u(\xi,\eta),w(\xi,\eta),\Lambda(\xi,\eta),\Psi(\xi,\eta))\\ &= K\int_0^T\int_0^1 r\overline{\overline{D_t^2\Psi}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)h(r)\,dr\,dt\\ &\quad +K\int_0^T\int_0^1 r\overline{\overline{D_t^2 u}}(r,q(r),t)\overline{\overline{\Lambda}}(r,q(r),t)h(r)\,dr\,dt. \qquad (2.25)\end{aligned}$$

(where the first equality follows from (2.17)) if the previous four equations are satisfied.

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Clearly, the third equation in (2.24) is an equation for u and the fourth equation is an equation for w. As expected, u and w are the results already obtained in (2.12), (2.13) for calculation of the first-order sensitivities. If we compare the second equation and (2.11), it turns out that the Lagrange multiplier Ψ is $\frac{d}{d\xi}u$. Finally, the first equation is an equation for Λ. It can be seen as the derivative of the adjoint state w with respect to ξ. (The first and the third equation can be derived by taking derivative with respect to ξ of the fourth and the third equation, respectively). In summary, second-order sensitivity analysis using an adjoint approach doesn't avoid calculation of the derivatives as in the case of the first order sensitivities. However, calculation of the second-order derivatives of the solution is avoided.

Analogously, one can compute

$$\begin{aligned}
\frac{\partial^2 j}{\partial \xi^2} &= K \int_0^T \int_0^1 r\overline{\overline{D_t^2 \Psi^s}}(r, q(r), t)\overline{\overline{w}}(r, q(r), t)s(r)\, dr\, dt \\
&\quad + K \int_0^T \int_0^1 r\overline{\overline{D_t^2 u}}(r, q(r), t)\overline{\overline{\Lambda^s}}(r, q(r), t)s(r)\, dr\, dt \\
\frac{\partial^2 j}{\partial \eta \partial \xi} &= K \int_0^T \int_0^1 r\overline{\overline{D_t^2 \Psi^h}}(r, q(r), t)\overline{\overline{w}}(r, q(r), t)s(r)\, dr\, dt \\
&\quad + K \int_0^T \int_0^1 r\overline{\overline{D_t^2 u}}(r, q(r), t)\overline{\overline{\Lambda^h}}(r, q(r), t)s(r)\, dr\, dt \\
\frac{\partial^2 j}{\partial \eta^2} &= K \int_0^T \int_0^1 r\overline{\overline{D_t^2 \Psi^h}}(r, q(r), t)\overline{\overline{w}}(r, q(r), t)h(r)\, dr\, dt \\
&\quad + K \int_0^T \int_0^1 r\overline{\overline{D_t^2 u}}(r, q(r), t)\overline{\overline{\Lambda^h}}(r, q(r), t)h(r)\, dr\, dt,
\end{aligned} \tag{2.26}$$

where for the last two equalities, Ψ and Λ solve appropriate equations with s replaced by h, as is indicated by Ψ^h and Λ^h in contrast to Ψ^s and Λ^s for the first two derivatives.

Remark 2.4.1 *For the full lens model (1.2), (1.3) with lower and upper surface parametrization q^l, q^u as well as the corner point (L, H) as design variables, the first partial derivatives are given by*

$$\frac{\partial J}{\partial q^u}[s] = K \int_0^T \int_0^L r\overline{\overline{D_t u D_t w}}\left(r, H + q^u\left(\frac{r}{L}\right), t\right) s(r)\, dr\, dt \tag{2.27}$$

$$\frac{\partial J}{\partial q^l}[s] = K \int_0^T \int_0^L r\overline{\overline{D_t u D_t w}}\left(r, H + q^l\left(\frac{r}{L}\right), t\right) s(r)\, dr\, dt \tag{2.28}$$

$$\begin{aligned}
\frac{\partial J}{\partial H} &= K \int_0^T \int_0^L r\Bigg(\overline{\overline{D_t u D_t w}}\left(r, H + q^u\left(\frac{r}{L}\right), t\right) \\
&\quad - \overline{\overline{D_t u D_t w}}\left(r, H + q^l\left(\frac{r}{L}\right), t\right)\Bigg)\, dr\, dt
\end{aligned} \tag{2.29}$$

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$$\frac{\partial J}{\partial L} = -\frac{1}{L^2} K \int_0^T \int_0^L r \left(\overline{\overline{D_t u D_t w}} \left(r, H + q^u \left(\frac{r}{L} \right), t \right) q^{u'}(r) \right.$$
$$\left. - \overline{\overline{D_t u D_t w}} \left(r, H + q^l \left(\frac{r}{L} \right), t \right) q^{l'}(r) \right) dr\, dt. \tag{2.30}$$

3 Nonlinear model for the lithotripter

In contrast to the previous section, where for modelling ultrasound propagation we used the linear acoustic wave equation, we will now build a similar model based on an equation in nonlinear acoustics.

3.1 PDE

The equation we are going to use here is the Westervelt equation of nonlinear acoustics. More precisely, we will consider the following initial-boundary value problem:

$$\begin{aligned} -\frac{1}{c^2} D_t^2 u + \Delta u + \frac{b}{c^2} \Delta (D_t u) &= -\frac{\beta_a}{\rho c^4} D_t^2 u^2 \quad \text{in } (0,T) \times \Omega \\ \frac{\partial u}{\partial n} &= g \quad \text{on } (0,T) \times \Gamma_0 \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } (0,T) \times (\partial\Omega \setminus \Gamma_0) \\ u(0,\cdot) = D_t u(0,\cdot) &= 0 \quad \text{in } \Omega. \end{aligned} \tag{3.1}$$

Here, as before, u is the acoustic pressure, c is the speed of sound, b is the diffusivity of the sound, ρ is the mass density and β_a is the parameter of nonlinearity.

Remark 3.1.1 *For the sake of simplicity, we do not assume here the absorbing boundary conditions as in the linear case. However, it is easy to see that it would only introduce one additional boundary term on the left-hand side of the following equations.*

We introduce an abbreviation $k = \frac{\beta_a}{\rho c^2}$ and assume that coefficients of the equation are piecewise constant

$$c(x) = \begin{cases} c_s & x \in \Omega_s \\ c_f & x \in \Omega_f \end{cases} \quad b(x) = \begin{cases} b_s & x \in \Omega_s \\ b_f & x \in \Omega_f \end{cases} \quad k(x) = \begin{cases} k_s & x \in \Omega_s \\ k_f & x \in \Omega_f \end{cases} \tag{3.2}$$

Now, the weak form of the PDE is given by

$$\begin{aligned} &\int_\Omega D_t^2 u w\, dx + \int_\Omega \nabla u \nabla (c^2 w)\, dx + \int_\Omega \nabla (D_t u) \nabla (b w)\, dx - \int_\Omega k D_t^2 u^2 w\, dx \\ &= \int_{\Gamma_0} (c_f^2 g + b_f D_t g) w\, d\Gamma, \quad \forall w \in L^2(0,T; H^1(\Omega)) \\ &\qquad\qquad u(0,\cdot) = u_0, \qquad D_t u(0,\cdot) = u_1 \end{aligned} \tag{3.3}$$

$u \in \widetilde{W}(0,T) = \{u \in L^\infty((0,T) \times \Omega) \mid u, D_t u \in H^1((0,T) \times \Omega))\}$, see, [3].

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Remark 3.1.2 *This formulation is correct only under additional assumption that*

$$\int_{\Gamma_s} \left(c_s^2 \frac{\partial u_s}{\partial \nu} w_s - c_f^2 \frac{\partial u_f}{\partial \nu} w_f + b_s \frac{\partial D_t u_s}{\partial \nu} w_s - b_f \frac{\partial D_t u_f}{\partial \nu} w_f \right) d\Gamma = 0 \tag{3.4}$$

holds for all $w \in H^1(\Omega)$, *where* $\Gamma_s = \partial\Omega_s$ *and* n *is the outward unit surface normal to* Γ_s *and* w_f, w_s *are the limits of* w *taken from inside of* Ω_f, Ω_s, *respectively. Since* $C^\infty(\Omega)$ *is dense in* $H^1(\Omega)$, *this implies that the interface condition*

$$c_s^2 \frac{\partial u_s}{\partial \nu} + b_s \frac{\partial D_t u_s}{\partial \nu} = c_f^2 \frac{\partial u_f}{\partial \nu} + b_f \frac{\partial D_t u_f}{\partial \nu}$$

holds, cf. [2] for the linear case without damping (i.e. $b_f = b_s = 0$*). Likewise, we also assume continuity of* u *over the interface* Γ_s.

Remark 3.1.3 *We also assume that (3.3) is uniquely solvable for given initial and boundary data. For coefficients* c, b, k, *that are constant on the whole domain, this has been shown in [13]. For the piecewise constant case we are considering here, it is still work in progress.*

3.2 Sensitivity analysis

3.2.1 *Derivative of u with respect to q*

Similarly as for the linear case, we obtain

$$\begin{aligned}
&\int_\Omega D_t^2 v^s w \, dx + \int_\Omega \nabla v^s \nabla(c^2 w) \, dx + \int_\Omega \nabla(D_t v^s) \nabla(bw) \, dx - 2 \int_\Omega k D_t^2 (u v^s) w \, dx \\
&\quad = -K_1 \int_0^1 r \overline{\overline{\Delta u}}(r, q(r), t) \overline{\overline{w}}(r, q(r)) s(r) \, dr \\
&\qquad - K_2 \int_0^1 r \overline{\overline{\Delta (D_t u)}}(r, q(r), t) \overline{\overline{w}}(r, q(r)) s(r) \, dr \\
&\qquad - K_3 \int_0^1 r \overline{\overline{D_t^2 u^2}}(r, q(r), t) \overline{\overline{w}}(r, q(r)) s(r) \, dr \qquad \forall w \in H^1(\Omega),
\end{aligned} \tag{3.5}$$

where the constants are defined as $K_1 = 2\pi(c_f^2 - c_s^2)$, $K_2 = 2\pi(b_f - b_s)$, $K_3 = 2\pi(k_f - k_s)$, and $v^s = \lim_{\varepsilon \to 0} \frac{u_\varepsilon^s - u}{\varepsilon}$, $u_\varepsilon^s = u(q + \varepsilon s)$.

Remark 3.2.1 *Here we also set* $L = 1, H = 0$ *and consider a single interface for the sake of simplicity.*

Since the Westervelt equation is given in terms of the acoustic pressure, we can use the same cost functional as in the linear case.

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3.2.2 *Derivative of j with respect to design parameter q*

The sensitivity analysis for the nonlinear problem can be performed in the same manner as for the linear one. So again, we consider the biparametric family of perturbations

$$q \mapsto q_{\xi\eta} = q + \xi s + \eta h,$$

where s and h are the directions of perturbation. We introduce the Lagrangian

$$\begin{aligned}\mathscr{L}(\xi,\eta;u,w) = J(u) &+ \int_0^T\int_\Omega D_t^2 uw\,dx\,dt + \int_0^T\int_\Omega \nabla u\nabla(c^2 w)\,dx\,dt \\ &+ \int_0^T\int_\Omega \nabla(D_t u)\nabla(bw)\,dx\,dt - \int_0^T\int_\Omega kD_t^2 u^2 w\,dx\,dt \\ &- \int_0^T\int_{\Gamma_0} (c_f^2 g + b_f D_t g)w\,d\Gamma\,dt \end{aligned} \tag{3.6}$$

and compute the variations with respect to its third and fourth variable to find

$$\begin{aligned}\langle D_u\mathscr{L}(\xi,\eta;u,w);v\rangle &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\mathscr{L}(\xi,\eta;u+\varepsilon v,w) - \mathscr{L}(\xi,\eta;u,w)) \\ &= 2\int_0^T\int_{\Omega_J}(u-u^d)v\,dx\,dt + \int_0^T\int_\Omega D_t^2 vw\,dx\,dt \\ &\quad + \int_0^T\int_\Omega \nabla v\nabla(c^2 w)\,dx\,dt + \int_0^T\int_\Omega \nabla(D_t v)\nabla(bw)\,dx\,dt \\ &\quad - 2\int_0^T\int_\Omega kD_t^2(uv)w\,dx\,dt, \\ \langle D_w\mathscr{L}(\xi,\eta;u,w);z\rangle &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\mathscr{L}(\xi,\eta;u,w+\varepsilon z) - \mathscr{L}(\xi,\eta;u,w)) \\ &= \int_0^T\int_\Omega D_t^2 uz\,dx\,dt + \int_0^T\int_\Omega \nabla u\nabla(c^2 z)\,dx\,dt \\ &\quad + \int_0^T\int_\Omega \nabla(D_t u)\nabla(bz)\,dx\,dt - \int_0^T\int_\Omega kD_t^2 u^2 z\,dx\,dt \\ &\quad - \int_0^T\int_{\Gamma_0}(c_f^2 g + b_f D_t g)z\,d\Gamma\,dt. \end{aligned} \tag{3.7}$$

If the following two equations are satisfied

$$\begin{aligned}\langle D_u\mathscr{L}(\xi,\eta;u,w);v\rangle &= 0 \quad \forall v \in L^2(0,T;H^1(\Omega)) \\ \langle D_w\mathscr{L}(\xi,\eta;u,w);z\rangle &= 0 \quad \forall z \in L^2(0,T;H^1(\Omega)) \end{aligned} \tag{3.8}$$

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we can conclude that for $j(q) = J(u(q))$

$$\begin{aligned}
\frac{\partial j}{\partial \xi} &= \frac{dJ(u(\xi,\eta))}{d\xi} = D_\xi \mathscr{L}(\xi,\eta;u(\xi,\eta),w(\xi,\eta)) \\
&= -K_1 \int_0^T \int_0^1 r\overline{\overline{\Delta u}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad - K_2 \int_0^T \int_0^1 r\overline{\overline{\Delta(D_t u)}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad - K_3 \int_0^T \int_0^1 r\overline{\overline{D_t^2 u^2}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&= -K_1 \int_0^T \int_0^1 r\overline{\overline{\Delta u}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad + K_2 \int_0^T \int_0^1 r\overline{\overline{\Delta u}}(r,q(r),t)\overline{\overline{D_t w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad + K_3 \int_0^T \int_0^1 r\overline{\overline{D_t u^2}}(r,q(r),t)\overline{\overline{D_t w}}(r,q(r),t)s(r)\,dr\,dt. \qquad (3.9)
\end{aligned}$$

As in the linear case, the first of the two equations in (3.8) is the weak form of the adjoint problem, which in its strong form reads as follows:

$$\begin{aligned}
D_t^2 w - \Delta(c^2 w) + D_t\Delta(bw) - 2kuD_t^2 w &= -2(u-u^d)\chi_{\Omega_J} \quad \text{in } (0,T)\times\Omega \\
\frac{\partial w}{\partial n} &= 0 \quad \text{on } (0,T)\times\partial\Omega \\
w(T,\cdot) = D_t w(T,\cdot) &= 0 \quad \text{in } \Omega.
\end{aligned}$$

For the second-order sensitivities, we introduce the second-order Lagrangian

$$\begin{aligned}
\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi) &= \frac{d}{d\xi}\mathscr{L}(\xi,\eta;u,w) + \langle D_u\mathscr{L}(\xi,\eta;u,w);\Psi\rangle + \langle D_w\mathscr{L}(\xi,\eta;u,w);\Lambda\rangle \\
&= -K_1 \int_0^T \int_0^1 r\overline{\overline{\Delta u}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad - K_2 \int_0^T \int_0^1 r\overline{\overline{\Delta(D_t u)}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad - K_3 \int_0^T \int_0^1 r\overline{\overline{D_t^2 u^2}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt \\
&\quad + 2\int_0^T \int_{\Omega_J} (u-u^d)\Psi\,dx\,dt + \int_0^T \int_\Omega D_t^2\Psi\, w\,dx\,dt + \int_0^T \int_\Omega \nabla\Psi\nabla(c^2 w)\,dx\,dt \\
&\quad + \int_0^T \int_\Omega \nabla(D_t\Psi)\nabla(bw)\,dx\,dt - 2\int_0^T \int_\Omega kD_t^2(u\Psi)w\,dx\,dt \\
&\quad + \int_0^T \int_\Omega D_t^2 u\Lambda\,dx\,dt + \int_0^T \int_\Omega \nabla u\nabla(c^2\Lambda)\,dx\,dt + \int_0^T \int_\Omega \nabla(D_t u)\nabla(b\Lambda)\,dx\,dt \\
&\quad - \int_0^T \int_\Omega kD_t^2 u^2\Lambda\,dx\,dt - \int_0^T \int_{\Gamma_0} (c_f^2 g + b_f D_t g)\Lambda\,d\Gamma\,dt. \qquad (3.10)
\end{aligned}$$

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Taking variations of $\mathscr{L}_2$ with respect to its third, fourth, fifth and sixth argument we obtain

$$\begin{aligned}\langle D_u\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);v\rangle = &-K_1\int_0^T\int_0^1 r\overline{\overline{\Delta v}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt\\ &-K_2\int_0^T\int_0^1 r\overline{\overline{\Delta(D_t v)}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt\\ &-2K_3\int_0^T\int_0^1 r\overline{\overline{D_t^2(uv)}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)s(r)\,dr\,dt\\ &+2\int_0^T\int_{\Omega_J} v\Psi\,dx\,dt-2\int_0^T\int_\Omega kD_t^2(v\Psi)w\,dx\,dt\\ &+\int_0^T\int_\Omega D_t^2 v\Lambda\,dx\,dt+\int_0^T\int_\Omega \nabla v\nabla(c^2\Lambda)\,dx\,dt\\ &+\int_0^T\int_\Omega \nabla(D_t v)\nabla(b\Lambda)\,dx\,dt-2\int_0^T\int_\Omega kD_t^2(uv)\Lambda\,dx\,dt \qquad (3.11)\end{aligned}$$

$$\begin{aligned}\langle D_w\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);z\rangle = &-K_1\int_0^T\int_0^1 r\overline{\overline{\Delta u}}(r,q(r),t)\overline{\overline{z}}(r,q(r),t)s(r)\,dr\,dt\\ &-K_2\int_0^T\int_0^1 r\overline{\overline{\Delta(D_t u)}}(r,q(r),t)\overline{\overline{z}}(r,q(r),t)s(r)\,dr\,dt\\ &-K_3\int_0^T\int_0^1 r\overline{\overline{D_t^2u^2}}(r,q(r),t)\overline{\overline{z}}(r,q(r),t)s(r)\,dr\,dt\\ &+\int_0^T\int_\Omega D_t^2\Psi z\,dx\,dt+\int_0^T\int_\Omega \nabla\Psi\nabla(c^2 z)\,dx\,dt\\ &+\int_0^T\int_\Omega \nabla(D_t\Psi)\nabla(bz)\,dx\,dt-2\int_0^T\int_\Omega kD_t^2(u\Psi)z\,dx\,dt \qquad (3.12)\end{aligned}$$

$$\begin{aligned}\langle D_\Lambda\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\lambda\rangle = &\int_0^T\int_\Omega D_t^2 u\lambda\,dx\,dt+\int_0^T\int_\Omega \nabla u\nabla(c^2\lambda)\,dx\,dt\\ &+\int_0^T\int_\Omega \nabla(D_t u)\nabla(b\lambda)\,dx\,dt-\int_0^T\int_\Omega kD_t^2u^2\lambda\,dx\,dt\\ &-\int_0^T\int_{\Gamma_0}(c_f^2 g+b_f D_t g)\lambda\,d\Gamma\,dt \qquad (3.13)\end{aligned}$$

$$\begin{aligned}\langle D_\Psi\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\psi\rangle = &2\int_0^T\int_{\Omega_J}(u-u^d)\psi\,dx\,dt+\int_0^T\int_\Omega D_t^2\psi w\,dx\,dt\\ &+\int_0^T\int_\Omega \nabla\psi\nabla(c^2 w)\,dx\,dt+\int_0^T\int_\Omega \nabla(D_t\psi)\nabla(bw)\,dx\,dt\\ &-2\int_0^T\int_\Omega kD_t^2(u\psi)w\,dx\,dt \qquad (3.14)\end{aligned}$$

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to deduce

$$\begin{aligned}\frac{\partial^2 j}{\partial\xi\partial\eta} &= \frac{d}{d\eta}\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi)\\ &= -K_1\int_0^T\int_0^1 r\overline{\overline{\Delta\Psi}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)h(r)\,dr\,dt\\ &\quad - K_2\int_0^T\int_0^1 r\overline{\overline{\Delta(D_t\Psi)}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)h(r)\,dr\,dt\\ &\quad - 2K_3\int_0^T\int_0^1 r\overline{\overline{D_t^2(u\Psi)}}(r,q(r),t)\overline{\overline{w}}(r,q(r),t)h(r)\,dr\,dt\\ &\quad - K_1\int_0^T\int_0^1 r\overline{\overline{\Delta u}}(r,q(r),t)\overline{\overline{\Lambda}}(r,q(r),t)h(r)\,dr\,dt\\ &\quad - K_2\int_0^T\int_0^1 r\overline{\overline{\Delta(D_t u)}}(r,q(r),t)\overline{\overline{\Lambda}}(r,q(r),t)h(r)\,dr\,dt\\ &\quad - K_3\int_0^T\int_0^1 r\overline{\overline{D_t^2u^2}}(r,q(r),t)\overline{\overline{\Lambda}}(r,q(r),t)h(r)\,dr\,dt\end{aligned}\tag{3.15}$$

provided the following equations

$$\begin{aligned}\langle D_u\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);v\rangle &= 0 \quad \forall v\in L^2(0,T;H^1(\Omega))\\ \langle D_w\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);z\rangle &= 0 \quad \forall z\in L^2(0,T;H^1(\Omega))\\ \langle D_\Lambda\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\lambda\rangle &= 0 \quad \forall \lambda\in L^2(0,T;H^1(\Omega))\\ \langle D_\Psi\mathscr{L}_2(\xi,\eta;u,w,\Lambda,\Psi);\psi\rangle &= 0 \quad \forall \psi\in L^2(0,T;H^1(\Omega))\end{aligned}\tag{3.16}$$

are satisfied.

4 Conclusions and outlook

We have presented two possibilities to model the problem of ultrasound focusing in lithotripsy. The first one is based on linear acoustics, the second one on the more advanced nonlinear Westervelt equation. For each of them we did the first- and second-order shape sensitivity analysis which can be used in numerical optimization methods.

An alternative possibility to approach Extracorporreal Shock Wave Lithotripsy is described in [3], where the model is based on optimal boundary controllability.

As indicated earlier, we want to extend the proposed models by considering acoustic-elastic coupling, where the propagation of ultrasound through the lens will be described by linear elastic wave equation. We are also working on a well-posedness proof for (3.1) with jumping coefficients c, b, k.

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Appendix A

For the sake of completeness, we here state theorem 2.10 from the book [9] which we have used in Section 2.3.

To this end, let $\mathcal{O}$ be a family of admissible domains and $\tilde{\mathcal{O}}$, a larger family of domains $\mathcal{O} \subset \tilde{\mathcal{O}}$, which can be used, e.g. for discretization purposes.

Then for a sequence of domains $\{\Omega_n\}, \Omega_n \in \tilde{\mathcal{O}}$ and $\Omega \in \tilde{\mathcal{O}}$, we denote that the sequence $\{\Omega_n\}$ tends to Ω by

$$\Omega_n \xrightarrow{\tilde{\mathcal{O}}} \Omega, \quad n \to \infty. \tag{A 1}$$

For the convergence in $\tilde{\mathcal{O}}$, we assume the usual property, namely that for any subsequence Ω_{n_k} of Ω_n we have that

$$\Omega_{n_k} \xrightarrow{\tilde{\mathcal{O}}} \Omega, \quad k \to \infty, \tag{A 2}$$

if (A 1) holds.

Now, for any $\Omega \in \tilde{\mathcal{O}}$, we introduce the space of real functions $H(\Omega)$. As for convergence of functions from $H(\Omega)$ for different $\Omega \in \tilde{\mathcal{O}}$, where y_n is a sequence of functions such that $y_n \in H(\Omega_n)$ and $\Omega_n \in \tilde{\mathcal{O}}$, and $y \in H(\Omega)$ with $\Omega \in \tilde{\mathcal{O}}$, we denote it by

$$y_n \rightsquigarrow y, \quad n \to \infty. \tag{A 3}$$

For the convergence of functions we assume the analogous property as for the domains with respect to subsequences.

On any $\Omega \in \tilde{\mathcal{O}}$ we consider a state problem, which is assumed to have a unique solution and therewith defines a mapping

$$u : \Omega \mapsto u(\Omega) \in H(\Omega), \quad \Omega \in \tilde{\mathcal{O}}. \tag{$\mathcal{P}(\Omega)$}$$

The graph $\mathcal{G}$ of the mapping u restricted to $\mathcal{O}$ is defined as $\mathcal{G} = \{(\Omega, u(\Omega)) \mid \Omega \in \mathcal{O}\}$ and the cost functional as $J : (\Omega, y) \mapsto J(\Omega, y) \in \mathbb{R}$ with $\Omega \in \tilde{\mathcal{O}}, y \in H(\Omega)$.

We can now introduce an optimal shape design problem in the abstract form as

$$\begin{cases} \text{Find } \Omega^* \in \mathcal{O} \text{ such that} \\ J(\Omega^*, u(\Omega^*)) \leqslant J(\Omega, u(\Omega)) \qquad \forall \Omega \in \mathcal{O}, \end{cases} \tag{$\mathbb{P}$}$$

where $u(\Omega) \in H(\Omega)$ solves $(\mathcal{P}(\Omega))$.

The existence of a solution to ($\mathbb{P}$) follows if we have a compactness-type property for graph $\mathcal{G}$ and a lower semicontinuity of the cost functional J, or more precisely
($\mathcal{B}1$) (*compactness of* $\mathcal{G}$) *for any sequence* $\{(\Omega_n, u(\Omega_n))\}$, $(\Omega_n, u(\Omega_n)) \in \mathcal{G}$, *there exists its*

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subsequence $\{(\Omega_{n_k}, u(\Omega_{n_k}))\}$ *and an element* $(\Omega, u(\Omega)) \in \mathscr{G}$ *such that*

$$\Omega_{n_k} \xrightarrow{\tilde{\mathscr{O}}} \Omega,$$

$$u(\Omega_{n_k}) \rightsquigarrow u(\Omega), \quad k \to \infty;$$

($\mathscr{B}2$) (*lower semicontinuity of* J)

$$\left.\begin{array}{l} \Omega_n \xrightarrow{\tilde{\mathscr{O}}} \Omega,\ \Omega_n,\ \Omega \in \tilde{\mathscr{O}} \\ y_n \rightsquigarrow y,\ y_n \in H(\Omega_n),\ y \in H(\Omega) \end{array}\right\} \Rightarrow \liminf_{n\to\infty} J(\Omega_n, y_n) \geqslant J(\Omega, y).$$

Theorem A.0.2 *(theorem 2.10 in [9])*
Let ($\mathscr{B}1$) *and* ($\mathscr{B}2$) *be satisfied. Then* ($\mathbb{P}$) *has at least one solution.*

Idea of Proof. Property ($\mathscr{B}1$) guarantees existence of a convergent subsequence of a minimizing sequence, while property ($\mathscr{B}2$) implies optimality of its limit. □

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