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Raino A. E. Mäkinen

University of Jyväskylä
Department of Mathematical Information Technology
P.O. Box 35 (Agora)
FI–40014 University of Jyväskylä
FINLAND
fax +358 14 260 2771
http://www.mit.jyu.fi/

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On a Topology Optimization Problem Governed by the One-dimensional Wave Equation*

Raino A. E. Mäkinen†

Abstract

We formulate a topology optimization like problem for the one-dimensional time-harmonic wave equation. The wave equation is discretized using a mixed formulation. The time-periodic solution is obtained using an exact controllability approach. The optimization problem is solved using a gradient method utilizing exact sensitivities. Numerical examples are given.

1 Introduction

This paper discusses a design optimization problem governed by the wave equation. We concentrate on a material distribution / topology optimization like problem where a coefficient of the wave equation is sought to control the wave motion. Practical applications include e.g. electromagnetic band gap structures and photonic crystal waveguides [2], [6], [4], [9]. We consider the time-harmonic case but use a fully time-dependent mixed model. The periodity is obtained by an exact controllability approach.

The paper is organized as follows. In Section 2 we define the equations governing wave propagation in inhomogeneous media and their mixed finite element discretization; in Section 3 we formulate the design optimization problem, whereas sensitivity analysis and numerical realization issues are discussed in Sections 4 and 5, respectively. In Section 6 we demonstrate our approach with numerical examples dealing with design of band gap like structures.

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†Department of Mathematical Information Technology, University of Jyväskylä, PO Box 35 (Agora), FI-40014 University of Jyväskylä, Finland, raino.a.e.makinen@jyu.fi

2 The state problem

Consider the following wave equation in a truncated computational domain Ω (see Figure 1):

$$\begin{cases} \epsilon_r(x)\dfrac{\partial^2 u}{\partial t^2} - \nabla^2 u = 0 & \text{in } \Omega \times [0,T] \\ u_t + \nabla u \cdot \mathbf{n} = g & \text{on } \partial\Omega \times [0,T], \end{cases} \tag{1}$$

where the variable coefficient of the absolute term, given by

$$\epsilon_r(x) = \begin{cases} 1, & x \in \Omega \setminus \Omega_0 \\ 1 + q(x), & x \in \Omega_0,\ q \geq 0, \end{cases}$$

is used to model an inhomogeneity appearing inside Ω_0. On $\partial\Omega$, the condition is the simplest approximation of the combination of a non-reflecting boundary and external excitation. The problem (1) may model e.g. scattering of 3D acoustic or 2D polarized electric field.

We consider a time-periodic excitation g and solution to (1) with angular frequency ω and time-period $T = 2\pi/\omega$. The normal practise would be to re-write (1) as a complex valued Helmholtz equation. However, the solution of the Helmholtz problem is equivalent to finding a periodic solution of the original wave equation [1]. The T-periodic solution can be obtained by using the exact controllabily approach: the initial condition of the wave equation is adjusted in such a way that the solution and its time derivative coincides with the initial condition at time T.

Following [5] we define the following mixed exact controllability formulation of the time-periodic wave equation:

$$\epsilon_r v_t - \nabla \cdot \mathbf{p} = 0 \quad \text{in } \Omega \times [0,T] \tag{2}$$

$$\mathbf{p}_t - \nabla v = 0 \quad \text{in } \Omega \times [0,T] \tag{3}$$

$$v + c\mathbf{p} \cdot \mathbf{n} = g \quad \text{on } \partial\Omega \times [0,T] \tag{4}$$

$$v(0) = v(T) = e_0, \quad \mathbf{p}(0) = \mathbf{p}(T) = e_1 \quad \text{in } \Omega. \tag{5}$$

One immediately notices that the relation between (1) and (2)–(5) is the following:

$$v = u_t, \quad \mathbf{p} = \nabla u. \tag{6}$$

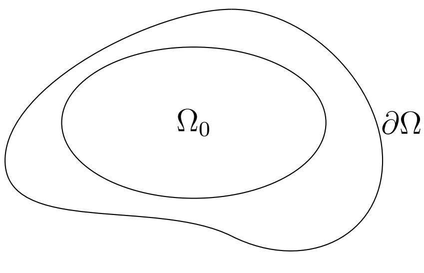

Figure 1: Problem geometry

Thus, the formulation has a flavor of a full 3D Maxwell system. This becomes more evident when using formulation in differential forms, as shown in [10].

In the rest of this paper we limit ourselves to the one-dimensional case

$$\epsilon_r \dot{v} - p_x = 0 \quad \text{in } Q \tag{7}$$

$$\dot{p} - v_x = 0 \quad \text{in } Q \tag{8}$$

$$v(0,t) - p(0,t) = g(t) \tag{9}$$

$$v(L,t) + p(L,t) = 0. \tag{10}$$

In order to perform the spatial discretization with the finite element method we derive the weak form of the system (7)–(10). By multiplying the equations (7) and (8) by test functions and performing integration by parts in the latter, the weak form

$$\int_0^L \epsilon_r \dot{v} w \, dx - \int_0^L p_x w \, dx = 0 \quad \forall w \in L^2(\Omega) \tag{11}$$

$$\int_0^L \dot{p} \psi \, dx + \int_0^L v \psi_x \, dx + p(L)\psi(L) + (p(0) + g(0))\psi(0) \quad \forall \psi \in H^1(\Omega). \tag{12}$$

is obtained.

Let $[0, L]$ be divided into $n - 1$ segments of length h. We perform the spatial discretization of (11)–(12) as follows

$$v_h(x,t) = \sum_{i=1}^{n-1} v_i(t) w_i(x), \quad p_h(x,t) = \sum_{i=1}^{n} p_i(t) \psi_i(x), \tag{13}$$

where $\{w_i\}_{i=1}^{n-1}$ are piecewise constant basis functions and $\{\psi_i\}_{i=1}^{n}$ are piecewise linear and continuous basis functions.

The semi-discretized wave equation can now be written in a matrix form as follows

$$\begin{bmatrix} \mathbf{M}_v & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_p \end{bmatrix} \begin{bmatrix} \dot{\mathbf{v}} \\ \dot{\mathbf{p}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & -\mathbf{B} \\ \mathbf{B}^{\mathrm{T}} & \mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{g} \end{bmatrix}, \tag{14}$$

where the "mass" matrix blocks are given by

$$\mathbf{M}_v = \text{diag}\left\{ h\epsilon_r((i - \tfrac{3}{2})h) \right\}_{i=2}^{n} \in \mathbb{R}^{(n-1)\times(n-1)},$$

$$\mathbf{M}_p = \text{diag}\left\{ \frac{h}{2}, h, h, ..., h, h, \frac{h}{2} \right\} \in \mathbb{R}^{n \times n}.$$

The blocks of the "stiffness/damping" matrix are given by

$$
\mathbf{B} = \begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & & \\ & & -1 & 1 & \\ & & & -1 & 1 \end{bmatrix} \in \mathbb{R}^{(n-1)\times n},
$$

$$
\mathbf{G} = \mathrm{diag}\{1, 0, 0, ..., 0, 0, 1\} \in \mathbb{R}^{n\times n},
$$

and the "forcing" vector by

$$
\mathbf{g} = [-g(0), 0, ..., 0]^{\mathrm{T}}.
$$

Denoting $\mathbf{y}{=}[\mathbf{v}\ \mathbf{p}]^{\mathrm{T}}$, $\mathbf{M}{=}\begin{bmatrix} \mathbf{M}_v & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_p \end{bmatrix}$, $\mathbf{K}{=}\begin{bmatrix} \mathbf{0} & -\mathbf{B} \\ \mathbf{B}^{\mathrm{T}} & \mathbf{G} \end{bmatrix}$, and $\mathbf{f}{=}[\mathbf{0}\ \mathbf{g}]^{\mathrm{T}}$ we can write the semidiscrete state problem shortly as follows:

$$
\begin{cases} \mathbf{M}\dot{\mathbf{y}} + \mathbf{K}\mathbf{y} = \mathbf{f} \\ \mathbf{y}(0) = \mathbf{y}(T). \end{cases} \tag{15}
$$

3 Optimization problem

Our aim is to design the coefficient function ϵ_r in such a way that the propagating wave has some desired property. We formulate the design optimization problem directly in a finite dimensional form. Define a partition

$$
x_i = a + (i-1)H,\ i = 1, ..., m, \quad H = (b-a)/m,
$$

where m and $0 < a < b < L$ are given. Then the parametrized coefficient function $\epsilon_r(\alpha; \cdot)$ is defined as follows

$$
\epsilon_r(\alpha; x) = \begin{cases} 1, & x < a \text{ or } x > b \\ 1 + \sum_{i=1}^{m} \alpha_i \phi_i(x) & \text{otherwise,} \end{cases} \tag{16}
$$

where $\phi_i = \chi_{[x_i, x_{i+1}[}$ (the characteristic function).

Then the semidiscrete ODE constrained design optimization problem can be written in abstract form as follows:

$$
\begin{cases} \text{Find } \alpha^* \in \mathcal{A} \quad \text{such that} \\ \mathcal{J}(\alpha^*, \mathbf{y}(\alpha^*)) \le \mathcal{J}(\alpha^*, \mathbf{y}(\alpha)) \quad \forall \alpha \in \mathcal{A}, \end{cases} \tag{17}
$$

where $\mathcal{A} = \{\alpha \in \mathbb{R}^m \mid \alpha_{\min} \le \alpha_i \le \alpha_{\max},\ i = 1, ..., m\}$ is the set of admissible design variable vectors, $\mathbf{y}(\alpha)$ solves (15) corresponding to $\epsilon_r(\alpha; \cdot)$, and

$$
\mathcal{J}(\alpha, \mathbf{v}) = \int_0^T G(\mathbf{v})\, dt + \beta \sum_{i=1}^{m} (\alpha_i - \alpha_{\min})(\alpha_{\max} - \alpha_i), \quad \beta \ge 0,
$$

is the cost functional.

Although the problem is formulated using a continuous control variable α, we would prefer an optimal control of a "bang-bang" type. Especially by choosing $\alpha_{\min} = 0$ the pure bang-bang solution would imply that $\epsilon_r(x) \in \{1, 1+\alpha_{\max}\}$. This corresponds to the classical topology optimization approach by Bendsøe et al. [2].

In the definition of $\mathcal{A}$ there is no volume fraction constraint unlike in typical structural topology optimization problems. To force the final solution to be "black and white", a penalty term is added in $\mathcal{J}$. The fixed parameter β controls the amount of penalization.

4 Sensitivity analysis

As our aim is to apply gradient-based optimization methods, the partial derivatives of the objective function with respect to design variables must be evaluated. We perform the algebraic sensitivity analysis using the standard adjoint method. Consider the Lagrangian

$$\mathcal{L}(\alpha, \mathbf{y}, \mathbf{p}, \lambda) = \int_0^T \left[G - \mathbf{p}^{\mathrm{T}}(\mathbf{M}\dot{\mathbf{y}} + \mathbf{K}\mathbf{y} - \mathbf{f})\right] \, dt + \lambda^{\mathrm{T}}(\mathbf{y}(0) - \mathbf{y}(T)) \tag{18}$$

corresponding to the ODE constrained minimization problem (17). As we are looking for the partial derivatives of the objective funtion with respect to design variables, we take variations of $\mathcal{L}$ with respect to α and $\mathbf{y}$:

$$\delta_\alpha \mathcal{L} = \int_0^T \left[\delta G - \mathbf{p}^{\mathrm{T}}(\delta \mathbf{M}\dot{\mathbf{y}} + \delta \mathbf{K}\mathbf{y} - \delta \mathbf{f}\right] dt \tag{19}$$

$$\delta_{\mathbf{y}} \mathcal{L} = \int_0^T \left[(\nabla_{\mathbf{y}} G)^{\mathrm{T}} \delta \mathbf{y} - \mathbf{p}^{\mathrm{T}}(\mathbf{M}\delta\dot{\mathbf{y}} + \mathbf{K}\delta\mathbf{y})\right] dt + \lambda^{\mathrm{T}}(\delta\mathbf{y}(0) - \delta\mathbf{y}(T)) \tag{20}$$

Setting $\delta_{\mathbf{y}}\mathcal{L} = 0$ and moving the time derivative from $\delta\mathbf{y}$ to $\mathbf{p}$ using the integration by parts, we obtain the adjoint equation

$$\begin{cases} -\mathbf{M}\dot{\mathbf{p}} + \mathbf{K}^{\mathrm{T}}\mathbf{p} = \nabla_y G \\ \mathbf{p}(0) = \mathbf{p}(T). \end{cases} \tag{21}$$

The adjoint equation has periodic boundary conditions too but it is solved "backward" in time.

As $\mathbf{K}$ and $\mathbf{f}$ do not depend explicitly on the design, we finally have

$$\frac{\partial \mathcal{J}}{\partial \alpha_k} = -\int_0^T \mathbf{p}^{\mathrm{T}} \frac{\partial \mathbf{M}}{\partial \alpha_k} \dot{\mathbf{y}}, \quad k = 1, ..., m. \tag{22}$$

5 Numerical realization

Next we discuss on finding time-harmonic solution to the primal and adjoint state problems by exact controllability method. Consider the following initial value problem

$$\mathbf{M}\dot{\mathbf{y}} + \mathbf{K}\mathbf{y} = \mathbf{f}, \quad \mathbf{y}(0) = \mathbf{w}. \tag{23}$$

The exact controllability problem related to it reads:

$$\begin{cases} \text{Find } \mathbf{w} \in \mathbb{R}^N \text{ such that the solution to (23) satisfies} \\ \mathbf{y}(0) = \mathbf{w},\ \mathbf{y}(T) = \mathbf{w}. \end{cases} \tag{24}$$

Consider the following two initial value problems

$$\begin{cases} \mathbf{M}\dot{\mathbf{y}}_f + \mathbf{K}\mathbf{y}_f = \mathbf{f} \\ \mathbf{y}_f(0) = \mathbf{0} \end{cases} \tag{25}$$

and

$$\begin{cases} \mathbf{M}\dot{\mathbf{y}}_0 + \mathbf{K}\mathbf{y}_0 = \mathbf{0} \\ \mathbf{y}_0(0) = \mathbf{w} \end{cases} \tag{26}$$

Then the solution to (23) is given by

$$\mathbf{y}(t) = \mathbf{y}_0(t) + \mathbf{y}_f(t) = \exp(-t\mathbf{A})\mathbf{w} + \mathbf{y}_f,$$

where $\mathbf{A} = \mathbf{M}^{-1}\mathbf{K}$. The exact controllability problem (24) can now be formulated as a linear system of equations

$$\left(e^{-T\mathbf{A}} - \mathbf{I}\right)\mathbf{w} = -\mathbf{y}_f(T). \tag{27}$$

We discuss later how this can be realized in practical computations.

Similarly, in the case of the adjoint equation (21), the two auxiliary intial value problems are

$$\begin{cases} -\mathbf{M}\dot{\mathbf{p}}_f + \mathbf{K}^T\mathbf{p}_f = \nabla_{\mathbf{y}}G \\ \quad \mathbf{p}_f(T) = \mathbf{0} \end{cases} \tag{28}$$

and

$$\begin{cases} -\mathbf{M}\dot{\mathbf{p}}_0 + \mathbf{K}^T\mathbf{p}_0 = \mathbf{0} \\ \quad \mathbf{p}_0(T) = \mathbf{q} \end{cases} \tag{29}$$

and the time-periodic solution

$$\mathbf{p}(t) = \mathbf{p}_0(t) + \mathbf{p}_f(t) = \exp(t\tilde{\mathbf{A}})\mathbf{q} + \mathbf{p}_f(t)$$

can be obtained by solving

$$\left(e^{T\tilde{\mathbf{A}}} - \mathbf{I}\right)\mathbf{q} = -\mathbf{p}_f(0), \tag{30}$$

where $\tilde{\mathbf{A}} = \mathbf{M}^{-1}\mathbf{K}^{\mathrm{T}}$.

In the numerical realization, the matrices $\mathcal{D} := e^{T\mathbf{A}} - \mathbf{I}$ and $\tilde{\mathcal{D}} := e^{T\tilde{\mathbf{A}}} - \mathbf{I}$ are not explicitly formed. The systems (27) , (30) can be solved using e.g. the restarted GMRES(k) method. The matrix-vector products of the form $\mathbf{y}^{(k)} = \mathcal{D}\mathbf{w}^{(k)}$ are computed by solving the initial value problems numerically with the fourth order Runge–Kutta method. Similarly, the time-integration in the cost function and its derivative with respect to design is evaluated using numerical integration.

We choose the element size as $h\omega = c_1 = \text{const}$. To satisfy the CFL condition, the time step is chosen as $\Delta t/h = c_2 = \text{const}$. Now, to solve the wave equation on $[0, T]$, the number of time-steps required is $K = 2\pi/\omega\Delta t$. With the previous choices of h and Δt, it follows that $K = 2\pi/c_1c_2$, i.e. independent on h and ω. Thus the computational cost of one GMRES iteration essentially equals to the cost of sparse matrix–vector multiply, i.e. $\mathcal{O}(N)$, where $N \sim 1/h$ is the number of degrees of freedoms.

In papers [3], [5], [7] the controllability problem (24) was solved in a different way. Instead of the non-symmetric sysmtem $\mathcal{D}\mathbf{w} = -\mathbf{y}_f(T)$ the symmetric system of "normal equation" $\mathcal{D}^{\mathrm{T}}\mathcal{D}\mathbf{w} = -\mathcal{D}^{\mathrm{T}}\mathbf{y}_f(T)$ was solved using the conjugate gradient method.

6 Numerical examples

In this section we present some numerical examples dealing with the optimization of band gap like structures to confirm the usefulness of the proposed method. All computations are realized in Matlab [8]. In optimization `fmincon` with `'sqp'` option from the MATLAB Optimization Toolbox was used.

In all examples the length of the computational domain is $L = 1$ and the function G defining the cost function is $G(v)(t) = \frac{1}{2}v(L,t)^2$, i.e., we are looking for a design that blocks the time-harmonic wave from going through the structure.

6.1 Example

We chose the following parameters: $\omega = 8\pi$, $a = 0.2$, $b = 0.8$, $\alpha_{\min} = 0$, $\alpha_{\max} = 5$, $h = 1/200$, $m = 20$, and $\beta = 10^{-4}$. Performing 32 SQP iterations (33 function evaluations) resulted in the design and state solution shown in Figure 2. The initial and final cost was 3.97×10^1 and 1.17×10^{-2}, respectively. Note that a completely "black and white" design was obtained.

In Figure 3 we have plotted the number of GMRES(100) iterations as a function of design changes. There are considerable differences between the iterations counts corresponding to different designs. Also the adjoint equation seems to be harder to solve than the primal one.

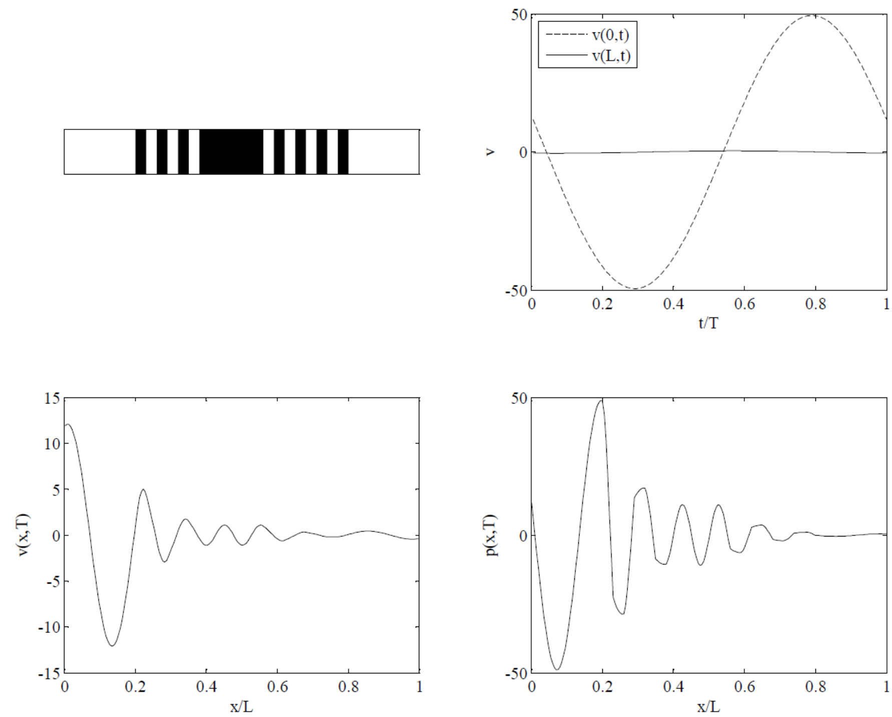

Figure 2: Top left: optimized structure. Top right: incoming and outcoming waves. Bottom: solution components (v, p) at $t = T$.

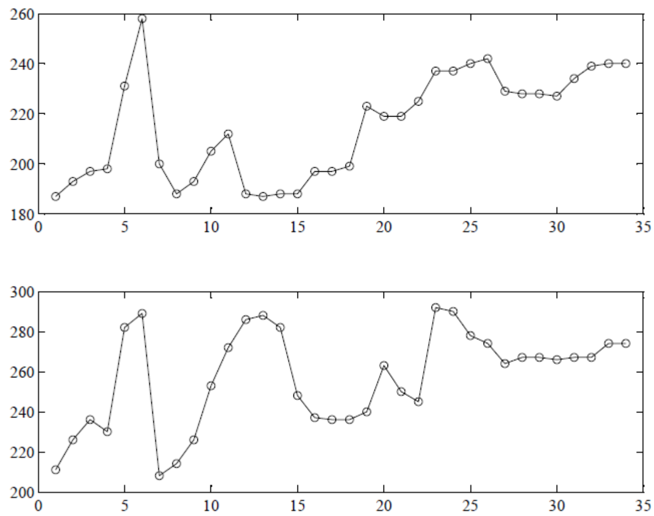

Figure 3: Number of GMRES iterations for the direct (top) and adjoint (bottom) problems.

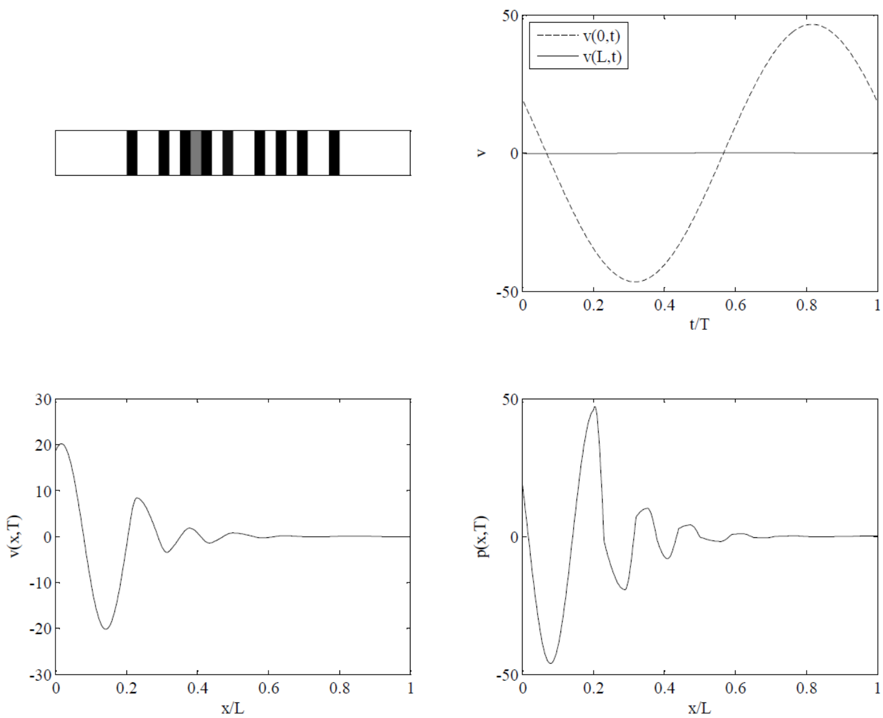

Figure 4: Top left: optimized structure. Top right: incoming and outcoming waves. Bottom: solution components (v, p) at $t = T$.

6.2 Example

The parameters defining the problem were kept the same as in Example 6.1, except that we chose a finer mesh with $h = 1/400$. Performing 54 SQP iterations (59 function evaluations) resulted in the design and state solution shown in Figure 4. The initial and final cost was 3.95×10^1 and 1.36×10^{-3}, respectively. In this case the design contains some gray elements. In Figure 5 we have plotted the number of GMRES(100) iterations as a function of design changes.

We then used the obtained design as an initial one for the same problem with bigger penalty parameter $\beta = 10^{-2}$. Performing 9 SQP iterations (10 function evaluations) resulted in the design and state solution shown in Figure 6. The initial and final cost was 7.87×10^{-2} and 8.74×10^{-4}, respectively.

7 Conclusions

In this paper we have demonstrated a "proof of concept" method to solve numerically a topology optimization problem governed by a wave equation. The method is based on solving the time-harmonic wave equation using exact controllability approach. The topology optimization is done using continuous variables. The "grey regions" are suppressed by adding a penalty term in the cost functional.

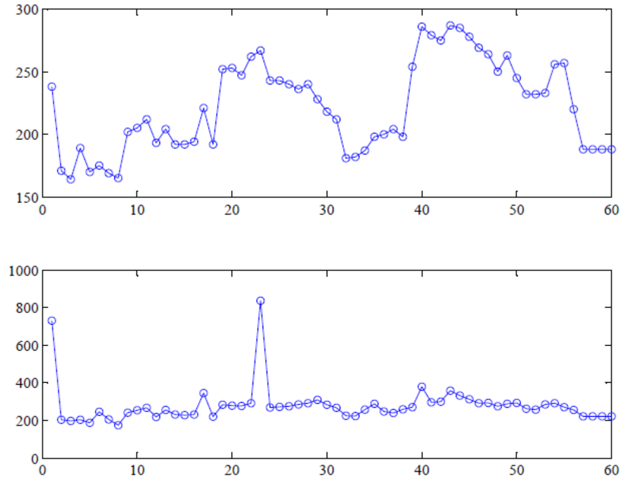

Figure 5: Number of GMRES iterations for the direct (top) and adjoint (bottom) problems.

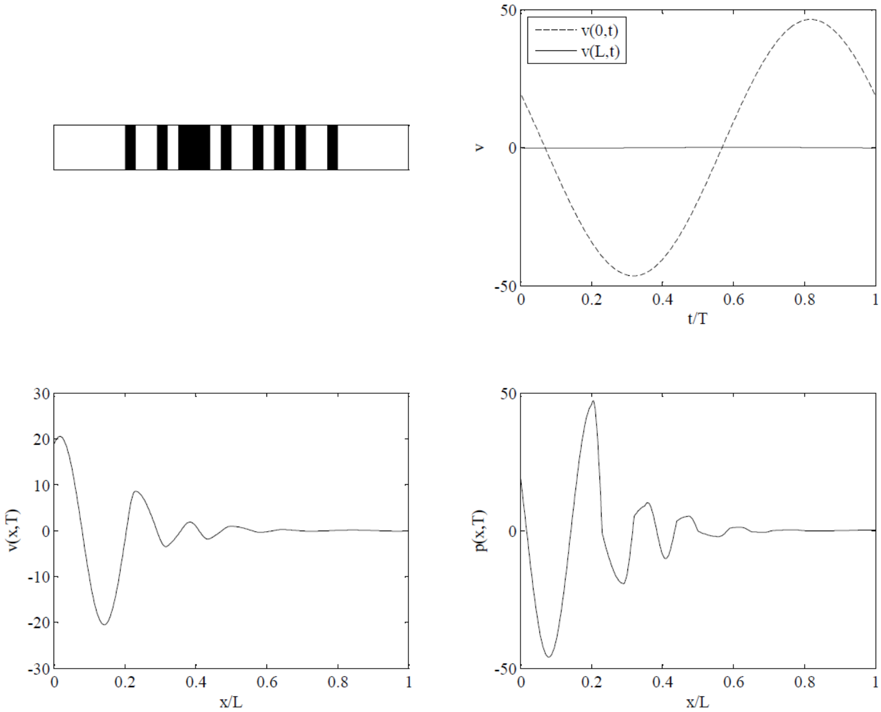

Figure 6: Top left: optimized structure. Top right: incoming and outcoming waves. Bottom: solution components (v, p) at $t = T$.

Although the 1D case is too simple to have significant practical use, it would be very interesting to apply this approach e.g. to time-harmonic Maxwell system in two or three dimensional setting.

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