Tracking optimization for propagation of electromagnetic waves for multiple wavelengths

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Abstract

The purpose of our work is to design dielectric composite structures with specific qualities. In this paper we construct interfaces of given material components such that the originated structure attains desired properties.

Propagation of the electromagnetic waves in the composite is described by the Helmholtz equation. Quality of the structure for a given set of wavelengths is enumerated by the tracking functionals that are to be minimized. Interfaces of the given materials are parametrized by the cubic B-spline curves. The design variables are afterwards the positions of B-spline control points.

For cost functional evaluation one forward computation of the Helmholtz equation for each wavelength is needed. To get the sensitivity of the objective function we solve the backward (adjoint) equation.

Several numerical simulations are presented. Finally three different designs are discussed.

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1. Introduction

Propagation of electromagnetic waves may be described by the Maxwell's equations — four integral laws. From these laws we may derive the Helmholtz equation for the Hertz potential (we have to make several assumptions - constitutive relations, time harmonics and further, see [1]).

Heterogeneities are distributed in the form of fibers — cylinders, we assume transverse-electric polarized waves. The state problem then becomes two dimensional and the Hertz potential is a scalar vector field defined within the domain Ω that is a bounded connected set in $\mathbb{R}^2$.

The medium of the scatterer and matrix is characterized by the complex refractive index. Our aim is to design shells of the scatterer in such a way that the resulting structure has a minimal influence on the incident planar wave (in the sense of the cost functional) across the given wavelength interval.

2. Problem setting

2.1. Description of the geometry

The geometry of the problem is described by figure 1. The state equation is considered in a rectangular domain $\overline{\Omega} = \sum_{i=1}^{11} \overline{\Omega}_i$ with the border $\Gamma^{11} = \Gamma_{in} \cup \Gamma_{out} \cup \Gamma_{up} \cup \Gamma_{low}$.

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We place a particle of certain properties in the middle of the computational domain. Its body is included in the set $\overline{\Omega}_1$ with the boundary Γ^1. The particle is enclosed by two layers and six smaller particles - domains $\Omega_2, \ldots, \Omega_9$ with the interfaces $\Gamma_d = \cup_{i=2}^9 \Gamma^i$. Interface curves Γ^i, $i = 2, \ldots, 9$ may vary and will be subject to shape optimization.

The refractive index is supposed to be constant in each subdomain of Ω, but is changing across interfaces.

The subdomain $\Omega_C := \Omega_{10}$ will be the support of the objective function.
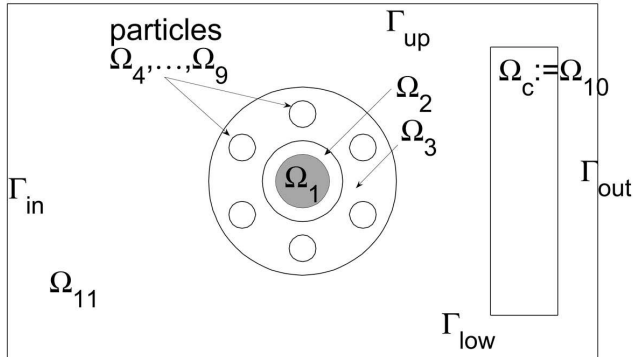

Fig. 1. Description of the geometry in 2D

2.2. State problem

Propagation of electromagnetic waves is described by the Helmholtz equation which is considered in the bounded domain $\Omega \subset \mathbb{R}^2$ (fig. 1). The planar wave with a given wavenumber k^{inc} comes through Γ_{in} and it proceeds further to the boundary Γ_{out}.

Amplitude A of the Hertz potential solves the state equation (cf. [1]):

$$
\begin{cases}
\dfrac{\partial^2 A}{\partial x_j \partial x_j} + k^2 A & = 0 & \text{in } \Omega, \\[2mm]
-\mathrm{j}kA + \dfrac{\partial A}{\partial x_j}n_j & = -2\beta \mathrm{j}k^{inc}\mathrm{e}^{-\mathrm{j}k^{inc}\mathbf{xn}} & \text{on } \Gamma_{in}, \\[2mm]
-\mathrm{j}kA + \dfrac{\partial A}{\partial x_j}n_j & = 0 & \text{on } \Gamma_{out}, \\[2mm]
\dfrac{\partial A}{\partial x_j}n_j & = 0 & \text{on } \Gamma_{up\&low},
\end{cases}
\tag{1}
$$

where $\beta \in \mathbb{R}$ is a given constant, $k = k(\mathbf{x}, \lambda)$ is the wavenumber, j is the imaginary unit, $\mathbf{n}$ is the outer unit normal vector and we have used the Einstein summation rule for the repeated indices.

The size of the computational domain should be sufficiently large, such that the boundary conditions are valid. Typically the outer boundary should be at least one wavelength far from the particle (that is in this case 500 nm). Detailed discussion of the boundary conditions in (1) may be found in [5].

The state equation in a weak form is defined as follows: Find the potential $A \in H(\Omega)$ that fulfills

$$-\int_\Omega \frac{\partial A}{\partial x_j} \frac{\partial \overline{\phi}}{\partial x_j}\, \mathrm{d}S + \int_\Omega k^2 A \overline{\phi}\, \mathrm{d}S + \mathrm{j} \int_{\Gamma_{in} \cup \Gamma_{out}} k A \overline{\phi}\, \mathrm{d}l = 2\mathrm{j}k^{inc} \int_{\Gamma_{in}} \beta \mathrm{e}^{-\mathrm{j}k^{inc}\mathbf{x}\cdot\mathbf{n}} \overline{\phi}\, \mathrm{d}l \tag{2}$$

$$\forall \phi \in H(\Omega),$$

where ϕ are test functions from the standard Sobolev space

$$H(\Omega) = W^{1,2} = \left\{ v \mid v, \frac{\partial v}{\partial x_i} \in L^2(\Omega),\ i = 1, 2 \right\}. \tag{3}$$

The bar sign denotes the complex conjugate value.

For the next considerations we will use the following notation

$$a(u, v) = \int_\Omega \frac{\partial u}{\partial x_j} \frac{\partial \overline{v}}{\partial x_j}\, \mathrm{d}S, \tag{4}$$

$$b(u, v) = \int_\Omega u \overline{v}\, \mathrm{d}S, \tag{5}$$

$$\langle u, v \rangle_\Gamma = \int_\Gamma u \overline{v}\, \mathrm{d}l. \tag{6}$$

The weak formulation (2) then changes to

$$\begin{cases} \text{Find } A \in H(\Omega) \text{ such that for all } \phi \in H(\Omega) \text{ holds} \\ -a(A, \phi) + b(k^2 A, \phi) + \mathrm{j}\langle kA, \phi \rangle_{\Gamma_{in} \cup \Gamma_{out}} = 2\mathrm{j}k^{inc} \langle \beta \mathrm{e}^{-\mathrm{j}k^{inc}\mathbf{x}\cdot\mathbf{n}}, \phi \rangle_{\Gamma_{in}}. \end{cases} \tag{7}$$

2.3. Cost functional

The aim of the optimization is to minimize the scattered field for a selected interval of wavelengths. It can be achieved by the worst scenario approach: we shall minimize amplitudes of the scattered field observed in a defined region for the worst case wavelength. Therefore, we shall compute the scattered response for selected wavelengths and by changing the design we minimize the maximum averaged amplitude.

Let $\Lambda = \{\lambda_1, \ldots, \lambda_n\}$ be a set of given wavelengths. Let Γ_{ad} be a set of admissible shapes. The task is to find the optimal design $\Gamma_d \in \Gamma_{ad}$ that solves

$$\min_{\Gamma_d \in \Gamma_{ad}} \max_{\lambda \in \Lambda} \psi(A_\lambda), \tag{8}$$

where ψ is the tracking functional for a given wavelength

$$\psi(A_\lambda) = \frac{1}{|\Omega_C|} \int_{\Omega_C} \left(\mathrm{Re}\left\{ A_\lambda^{scat} \right\} \right)^2 \mathrm{d}S = \frac{1}{|\Omega_C|} \int_{\Omega_C} \left(\mathrm{Re}\left\{ A_\lambda^{inc} - A_\lambda \right\} \right)^2 \mathrm{d}S, \tag{9}$$

where A_λ^{inc} is the incident Hertz potential for a wavelength $\lambda \in \Lambda$ when no particle and layers are present.

3. Sensitivity analysis

In this section we derive the sensitivity formula of the functional $\psi(A_\lambda)$ for a given wavelength $\lambda \in \Lambda$ with the constraint given by the state equation (7). We will use the material derivative approach (for details see [3]).

3.1. Lagrangian and adjoint equations

The Lagrangian is defined as the sum of the objective function and the weak formulation of the state equation (7), where the test function ϕ is replaced by the Lagrange multiplier $B \in H(\Omega)$

$$
\begin{aligned}
\mathcal{L}(\Gamma_d, A, B) =& \psi(A) - a(A, B) + b(k^2 A, B) + \mathrm{j}\langle kA, B \rangle_{\Gamma_{in} \cup \Gamma_{out}} - \\
& - 2\mathrm{j}k^{inc}\langle \beta \mathrm{e}^{-\mathrm{j}k^{inc}\mathbf{x}\cdot\mathbf{n}}, B \rangle_{\Gamma_{in}}.
\end{aligned}
\tag{10}
$$

The functional forms in (10) depend on the geometry (i.e. on the design) and on the state variable, which itself depends on the design, being the solution of the state problem. Therefore, to differentiate in (10), we apply the total variation that is defined as the design variation plus the variation according to the state variable

$$
\delta\mathcal{L} = \delta_\tau\mathcal{L} + \delta_A\mathcal{L}.
\tag{11}
$$

Design variation δ_τ is the partial derivative w.r.t. the domain perturbation in the direction of a vector field $\mathbf{V}$ defined as (cf. [3])

$$
\begin{aligned}
\delta_\tau f_\Omega(A) &= \frac{\mathrm{d}}{\mathrm{d}\tau}\left(f_{\Omega_D(\tau)}(A)\right)_{\tau=0}, \\
\Omega_D(\tau) &= \Omega + \{\tau\mathbf{V}(\mathbf{x})\}, \mathbf{x} \in \Omega, \tau \in \mathbb{R},
\end{aligned}
\tag{12}
$$

where $f : H(\Omega) \to \mathbb{R}$ is a given functional. The field $\mathbf{V}$ realizes the shape variations and it should be chosen in some natural way depending on the parametrization of admissible shapes.

By the variation of the given functional f according to the state variable in the direction of $C \in H(\Omega)$ we mean

$$
\delta_A f(A; C) = \lim_{t \to 0} \frac{f(A + tC) - f(A)}{t}.
\tag{13}
$$

Then the variation of the Lagrangian is given as

$$
\begin{aligned}
\delta\mathcal{L}(\Gamma_d, A, B) =& -\delta_\tau a(A, B) + \delta_\tau b(k^2 A, B) + \delta_\tau \mathrm{j}\langle kA, B \rangle_{\Gamma_{in} \cup \Gamma_{out}} - \\
& - a(\delta A, B) + b(k^2 \delta A, B) + \mathrm{j}\langle k\delta A, B \rangle_{\Gamma_{in} \cup \Gamma_{out}} + \delta_A\psi(A) \circ \delta A.
\end{aligned}
\tag{14}
$$

The optimality conditions with respect to the state variable are given as

$$
\delta_A\mathcal{L}(\Gamma_d, A, B) \circ C = -a(C, B) + b(k^2 C, B) + \mathrm{j}\langle kC, B \rangle_{\Gamma_{in} \cup \Gamma_{out}} + \delta_A\psi(A) \circ C = 0 \\
\forall C \in H(\Omega).
\tag{15}
$$

These conditions are often called the adjoint or backward equations.

We set $C = \delta A$ in (15) and substitute in the relation for the Lagrangian variation (14). The term $\delta_\tau\mathrm{j}\langle kA, B \rangle_{\Gamma_{in} \cup \Gamma_{out}}$ in (14) vanish because curves $\Gamma_{out}, \Gamma_{in}$ don't depend on a change of the design.

Finally we take such triples (Γ_d, A, B) that the potential A fulfills the state equation and the Lagrange multiplier B satisfies the adjoint equation. The constraint given by the state equation in the definition of the Lagrangian (10) then vanishes. For the sensitivity holds

$$
\delta\psi = \delta\mathcal{L}(\Gamma_d, A, B) = -\delta_\tau a(A, B) + \delta_\tau b(k^2 A, B).
\tag{16}
$$

As already has been mentioned the choice of $\mathbf{V}$ should reflect the given problem. We assume the domain Ω being occupied by an elastic medium and the field $\mathbf{V} \in \mathbf{H}_0^1(\Omega)$ is then response to the unit perturbation of particular B-spline control points (see fig. 2).

Formulas for differentiation given in [3] provide us the final form of the sensitivity as follows

$$\delta\psi = \int_\Omega \frac{\partial A}{\partial x_l} \frac{\partial\overline{B}}{\partial x_j} \frac{\partial V_l}{\partial x_j}\, dS + \int_\Omega \frac{\partial A}{\partial x_j} \frac{\partial\overline{B}}{\partial x_k} \frac{\partial V_k}{\partial x_j}\, dS - \int_\Omega \frac{\partial A}{\partial x_j} \frac{\partial\overline{B}}{\partial x_j} \mathrm{div}\, \mathbf{V}\, dS + \int_\Omega kA\overline{B}\mathrm{div}\, \mathbf{V}\, dS. \tag{17}$$
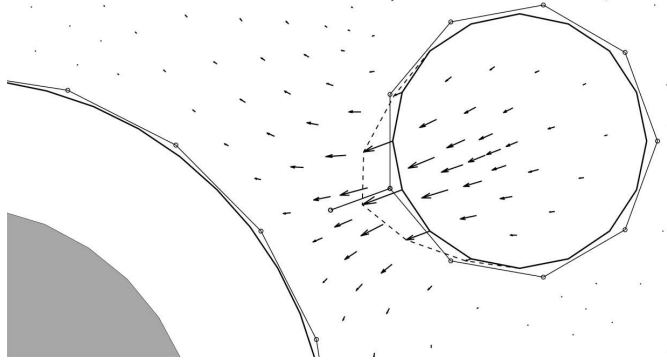

Fig. 2. Domain method: velocity field V — elastic displacement corresponding to the unit perturbation of the particular B-spline control point

3.2. Parametrization

For the definition of the design variation δ_τ we will need to parametrize the material interfaces. We use B-spline approximations ([4]) for their variability and relatively easy implementation.

Each design curve $\Gamma^j, j = 2, \dots, 9$ is parametrized by a closed cyclic B-spline of order $k = 4$ (cubic polynomial segments joined with C^2 continuity). If $(n_j + 1)$ is the number of control points corresponding to $\Gamma^j, j = 2, \dots, 9$, then the B-splines curves have the following form

$$\mathbf{X}^j(t, \mathbf{D}^j) = \sum_{i=0}^{n_j} \mathbf{d}_i^j N_{i4}(t) \quad t \in \left[t_3^j, t_{n_j+1}^j\right],$$
$$\mathbf{T}^j = (t_0^j, t_1^j, \dots, t_{n_j}^j, t_0^j, t_1^j, t_2^j, t_3^j), \tag{18}$$

where $\mathbf{D}^j$ is $(n_j + 1) \times 2$ matrix of $\mathbf{d}_i^j$ control points of the $j-$th curve, $N_{i4}(t)$ are basis-spline functions and $\mathbf{T}^j$ is the knot vector (for details see again [4]).

The choice of the control points may be done in the least squares sense (for details see [2]). Let $S^j = \left\{ \{t_i^j, \mathbf{p}_i^j\} \,|\, i = 0, \dots, r_j \right\}$ be the sets of $r_j + 1$ positions of finite element nodes $\mathbf{p}_i^j$ lying on the interfaces $j = 2, \dots, 9$ and t_i^j the corresponding parameters. For each curve Γ^j we wish to find the matrix $\mathbf{D}^{j*}$ that minimizes the value

$$c^j(\mathbf{D}^j) = \sum_{i=0}^{r_j} \left(\mathbf{p}_i^j - \mathbf{X}^j(t_i^j, \mathbf{D}^j) \right)^2,$$
$$\left\{ t_i^j, \mathbf{p}_i^j \right\} \in S^j. \tag{19}$$

Let us rewrite the B-splines representation in the matrix form

$$\mathbf{X}^j(t_i^j, \mathbf{D}^j) = \mathbf{A}_t^j \mathbf{D}^j, \tag{20}$$

where the matrix $\mathbf{A}_t^j$ (size $(r_j + 1) \times (n_j + 1)$) depends on the parameters t_i^j.

Let $\mathbf{P}^j := \left\{\mathbf{p}_i^j\right\}_{i=1}^{r_j}$, then the values c^j may be then written as

$$c^j(\mathbf{D}^j) = \text{trace}\left(\mathbf{P}^j - \mathbf{A}_t^j\mathbf{D}^j\right)^T \left(\mathbf{P}^j - \mathbf{A}_t^j\mathbf{D}^j\right). \tag{21}$$

The normal equations have the following form

$$\mathbf{A}_t^{jT}(\mathbf{A}_t^j\mathbf{D}^{j*} - \mathbf{P}^j) = \mathbf{0}, \tag{22}$$

where $\mathbf{D}^{j*}$ are the optimal positions of control points.

Finally from (22) we get

$$\mathbf{D}^{j*} = (\mathbf{A}_t^{jT}\mathbf{A}_t^j)^{-1}\mathbf{A}_t^{jT}\mathbf{P}^j. \tag{23}$$

This method enables us to use any initial shape of the design curves. The advantage of this approach becomes apparent also during the optimization process. After a few iterations very rugged shapes may develop. In that case remeshing is needed. Also the definition of new control points is suitable.

Once we have defined the parametrization of the design curves we may identify the design variables $\mathbf{l}_i^j$ as the parameters that define new positions of the B-spline control points

$$\mathbf{d}_i^j := \mathbf{d}_i^{j*} + \mathbf{l}_i^j, \tag{24}$$

where $\mathbf{d}_i^{j*}$ are the initial positions of control points defined by (23).

The set of admissible shapes is defined by the box constraints on the parameters $\mathbf{l}_i^j$

$$\Gamma_{ad} = \left\{\mathbf{l}_i^j | \mathbf{p}_i^j \leqq \mathbf{l}_i^j \leqq \mathbf{q}_i^j\right\}, \tag{25}$$

where $\mathbf{p}_i^j, \mathbf{q}_i^j$ are lower and upper bounds. On fig. 3 one of the admissible shapes may be seen.
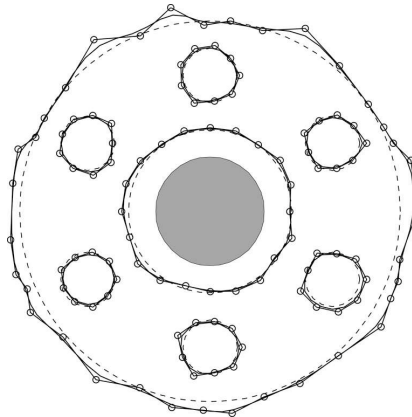

Fig. 3. B-splines approximation of the design curves, one of the admissible shapes

4. Implementation and results

4.1. Implementation

The discretization of the state equations was done by the classical approach of the finite element method (for details we recommend the well known book [6]). The state equation is solved by the finite element method using isoparametric, linear, triangular finite elements. On fig. 4 the implementation diagram is displayed.
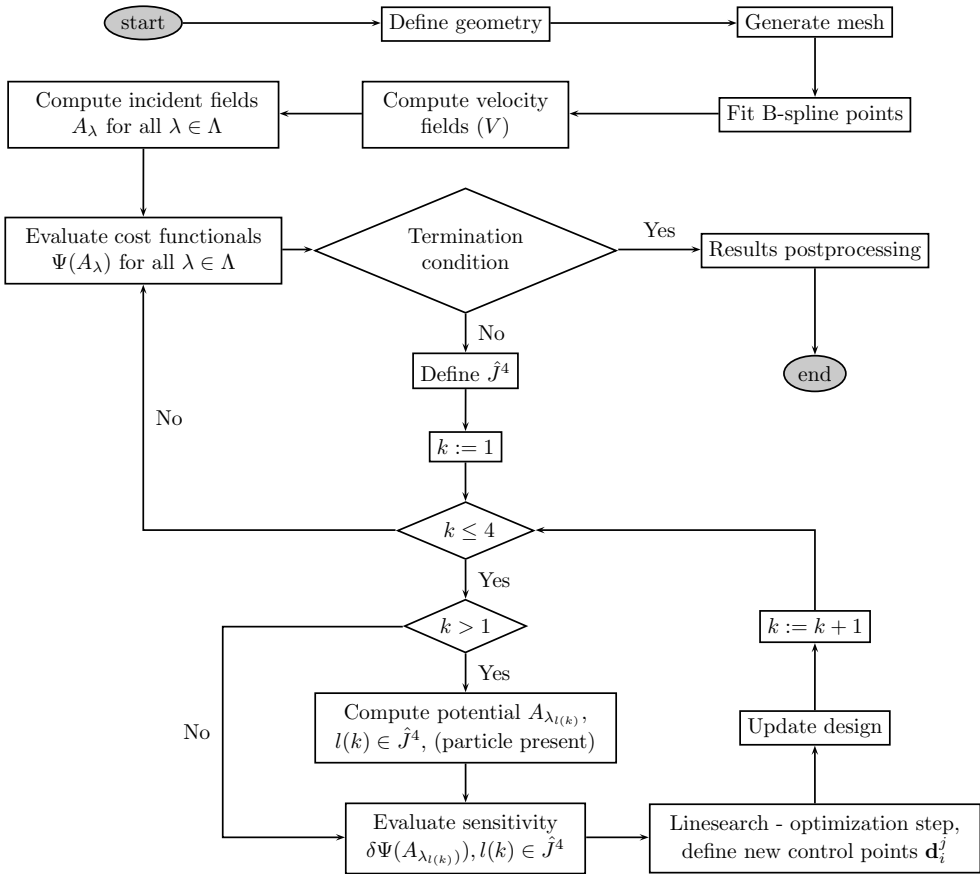

Fig. 4. Implementation diagram

To solve the min max problem (8) we have designed a heuristic algorithm. The algorithm contains two loops. In the outer loop we evaluate the cost functionals $\Psi(A_\lambda), \lambda \in \Lambda$. Further we pick up four highest values of the cost functionals and the corresponding wavelengths. That is, we define the set $\hat{J}^4$

$$\hat{J}^4 = \left\{ \{l(k)\}_{k=1}^4 \subset J \,|\, \Psi(A_{\lambda_j}) \leq \min_{k \in \{1,\ldots,4\}} \Psi(A_{\lambda_{l(k)}}) \,\forall j \in J \setminus \{l(k)\}_{k=1}^4 \right\}, \qquad (26)$$

where $J = \{1, \ldots, n\}$ is the index set of the wavelengths in Λ.

In the inner loop we optimize for the wavelengths given by $\hat{J}^4$.

The outer loop is running until the termination condition is fulfilled. The termination condition is defined by the constraint on the change of designs for last two successive iterations. If $\mathbf{d}_i^{j,r}, \mathbf{d}_i^{j,r-1}$ are the control points of the last two iterations of the outer loop, then the termination condition is given as follows

$$\sum_{i,j} \|\mathbf{d}_i^{j,r} - \mathbf{d}_i^{j,r-1}\|^2 < c, \tag{27}$$

where c is a given constant and $\| \cdot \|$ is the Euclidean norm in $\mathbb{R}^2$.

4.2. Numerical Simulations

We have performed several simulations for different geometries.

In first simulation (case 1) we optimized the particle with the initial shape given by the interrupted line in fig. 3. On fig. 5 you may see how the particle evolves towards the last iteration.

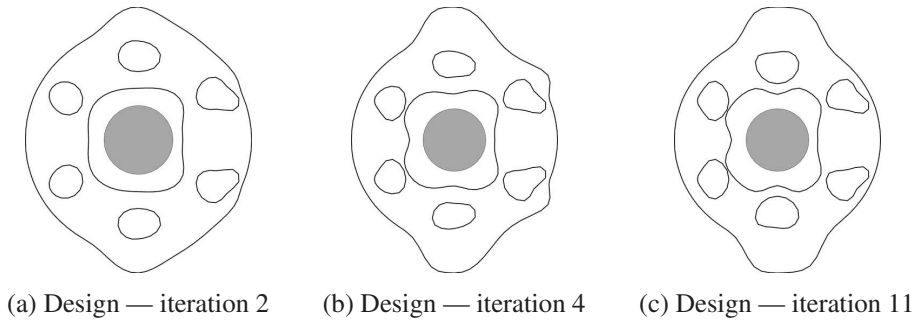| (a) Design — iteration 2 | (b) Design — iteration 4 | (c) Design — iteration 11 |

Fig. 5. Evolving design

On fig. 6 cost functional values corresponding to particular iteration are displayed. For higher iterations we have obtained no other improvements. We may observe that in average the final cost functional values are less than 50 % of their's initial values.
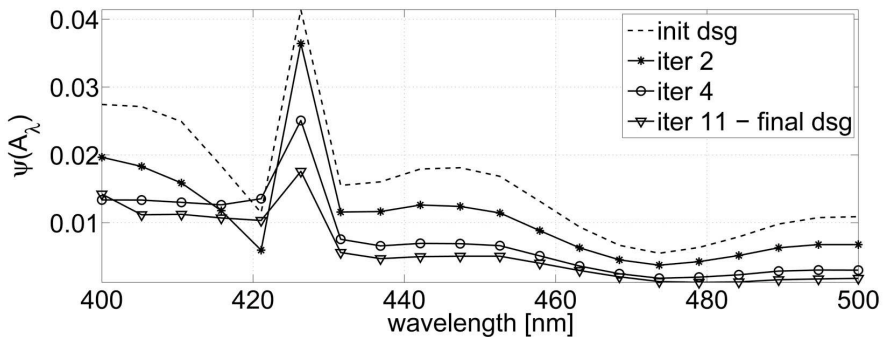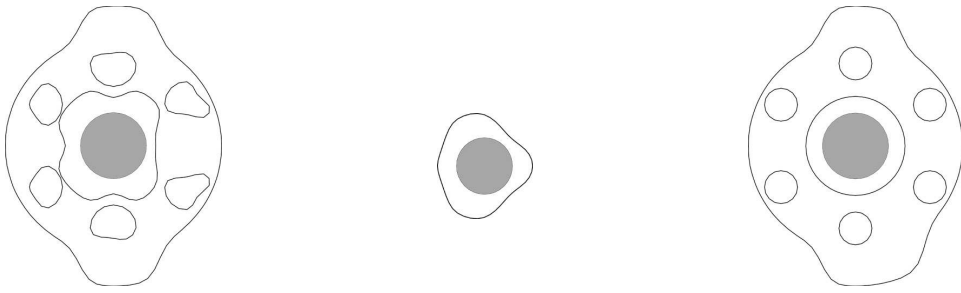

Fig. 6. Cost functional values for several iterations

(a) Design 1 — particles and layers are subject to optimization

(b) Design 2 — particle with one shell

(c) Design 3 — only outer layer may vary
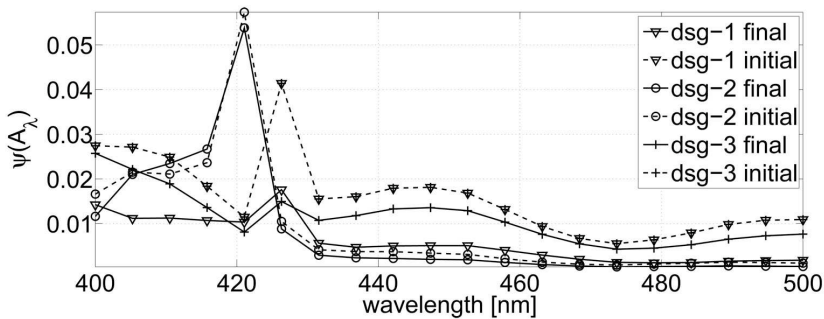
Fig. 7. Comparison of three different designs

Fig. 8. Initial and final cost functionals values for three considered designs

For comparison we have accomplished two other simulations. In the case 2 we have optimized the shape of the particle with just one shell. In the case 3 we have optimized the same particle as in the case 1, but we have allowed only variations of the outer shell. Final designs are displayed on fig. 7.

The initial and final cost functional values are displayed on fig. 8.

The results confirm that a more complex structure allows to obtain better gain from the optimization, i.e. to get a higher reduction of the cost function value w.r.t. that of the initial design.

5. Conclusion

We have proved that the cost functional is sensitive to the shape variations of the interface curves. Optimization provided us the structure which decreased the cost functional values more than over 50 %.

During the work there have arisen questions about the topology of the initial design — amount of shells, smaller particles and their's positions within the shells. The answers may be provided by means of the topology optimization. Topology gradient computation is the main aim we are focussed on currently. Further we consider modifications of the cost functional.

Acknowledgements

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