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Level set method with topological derivatives in shape optimization

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Abstract. A class of shape optimization problems is solved numerically by the level set method combined with the topological derivatives for topology optimization. Actually, the topology variations are introduced on the basis of asymptotic analysis, by an evaluation of extremal points (local maxima for the specific problem) of the so-called topological derivatives introduced by Sokolowski and Zochowski [24] for elliptic boundary value problems. Topological derivatives are given for energy functionals of linear boundary value problems. We present results, including numerical examples, which confirm that the application of topological derivatives in the framework of the level set method really improves the efficiency of the method. Examples show, that the level set method combined with the asymptotic analysis, is robust for the shape optimization problems, and it allows to identify the better solution compared to the *pure* level set method exclusively based on the boundary variation technique.

Key Words. Shape optimization, level set method, topological derivative, optimal design.

1. Introduction

Shape optimization for elliptic equations is an important branch of calculus of variations, with numerous applications in structural mechanics and to solution of inverse problems. The existence of solutions for shape optimization problems can be assured under mild conditions, e.g. under the so-called Mosco convergence of the Sobolev spaces associated with the minimizing sequence of geometrical domains, however optimality conditions require more regularity of boundaries of admissible domains. Recently, a particular attention is paid to numerical methods which during the optimization process allow for the topology changes of geometrical domains. One of the candidates for such framework is the level set function which models the domain evolution and can be determined by solving appropriate Hamilton-Jacobi equations. However, by its nature, the obtained level set function decreases the number of connected components of resulting geometrical domains during the optimization process. To improve the performance of the method based on the level set function, asymptotic analysis is employed, and location of additional holes in geometrical

domains is determined by analysis of the so-called topological derivatives of shape functionals under study. In the paper we describe in details such a combination, used already in literature, and provide some examples which show that the method is robust, in particular improves the *optimal* value of the shape functional obtained as a result of computations. For the convenience of the reader we present as well the elements of mathematical analysis including asymptotic analysis of specific boundary value problems with respect to small parameter which models singular perturbations of geometrical domains. Such analysis is required for determination of topological derivatives.

The numerical method for shape and topology optimization of an energy functional is presented in the paper. The method combines the shape gradient technique and the asymptotic analysis for maximization of an energy functional for elliptic equations. The level set method is used for the evolution of geometrical domains with the moving boundaries determined from the shape sensitivity analysis of the energy shape functional, the topology changes are performed in addition by analysis of the topological derivatives. It is still an open problem to devise how the combination of boundary variations and singular perturbations of geometrical domains enters in a general framework of shape optimization. One possibility is given by the so-called self-adjoint extensions of differential operators, where the small hole is approximated by singular perturbation of the coefficients of differential operator. We refer the reader to [18], [11], [14], [16], [17], for some results in this direction. We consider only steady state boundary value problems, however the same results can be obtained for the evolution problems described by parabolic and hyperbolic pde's.

The Hamilton-Jacobi nonlinear hyperbolic equation models the evolution of the level set function. The normal speed of the moving boundaries are determined from the shape gradients obtained for the energy functional [29]. Since the shape gradients serve as the coefficients for the hyperbolic equation, the standard assumption is to assume that the shape gradients are given by restriction to the moving boundaries of given functions defined in whole geometrical domains, which is unfortunately very restrictive assumption, however it is satisfied in our case.

During the numerical process, the topology changes are defined by analysis of the local maxima of topological derivatives for the energy functional. In this way, small holes can be included into the actual geometrical domain with the centers at the points determined by maximization of the topological derivatives. We inject only one hole at each etap of the method, however the asymptotic analysis furnish the information which allows for the injection of a finite number of holes, if necessary and it turns out to be useful. The size of the holes can be determined by the second order topological derivatives and this technique is not employed in the present paper.

The paper is selfcontained, thus, in appendix we provide also some technical results which are used in order to determine the topological derivatives. To this end the domain decomposition technique is applied and the proof of the asymptotic expansion for the related Steklov-Poincaré operator is given. Such an approach for evaluation of topological derivatives for energy type functionals is proposed e.g., in [12] and [27].

Finally, we present a list of references on the derivation and application of the asymptotic analysis in shape optimization. Singular perturbations of domains in the framework of shape optimization are studied by many authors, including [1], [9], [10], [13], [14], [15], [16], [17], [18], [19], [24], [25], [26]. The construction of the asymptotic expansion for the Steklov-Poincaré operator is given in [28]. Numerical results for shape and topology optimization are presented in section 9.

2. The linear problem

We present the numerical method for a scalar elliptic boundary value problems, and for the energy type shape functional. For such problem we can provide complete analysis on shape differentiation and asymptotic expansions of solutions with respect to small parameter which measures the singular perturbations of geometrical domain. For the sake of simplicity we restrict

ourselves to two spatial dimensions, and to the holes in the form of a circle. In such a case by Fourier analysis we can obtain the explicit solutions for auxiliary problems in rings. Otherwise, for any spatial dimensions and arbitrary shape of holes the analysis is based on the fundamental solutions for differential operators and can be performed in the same way, we refer the reader e.g., to [18] for a general approach to the derivation of topological derivatives for elliptic boundary value problems in arbitrary spatial dimensions.

To begin with, we introduce the model problem. Let U and V be two bounded open subsets of $\mathbb{R}^2$ such that $V \subset\subset U$. For any open set $\omega \subset \mathbb{R}^2$, we denote by $\#\overline{\omega}$ the number of connected components of $\overline{\omega}$ and we consider the set of admissible domains

$$\mathcal{O}_k = \{\Omega = U \setminus \overline{\omega};\ \omega \text{ open set},\ \omega \subset V, \#\overline{\omega} \leq k\}. \tag{1}$$

For any $\Omega \in \mathcal{O}_k$, $k \geq 1$, the boundary of Ω can be splitted into $\partial\Omega = \Gamma_N \cup \partial U$ with $\Gamma_N = \partial\omega$. The boundary ∂U is also denoted by Γ_D. The boundary Γ_N receives Neumann boundary conditions, while we have Dirichlet conditions on Γ_D. Let us point out that the open set ω is not necessarily any connected set as illustrated in Figure 1.

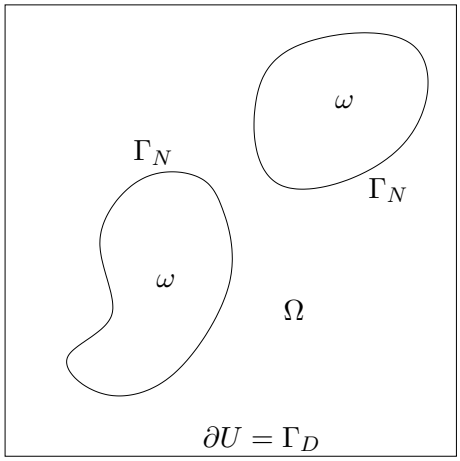

FIG. 1 – An admissible domain Ω

For $f \in C^\infty(\overline{U})$, let us consider the following problem

$$\left\{ \begin{array}{rcll} -\Delta u + u & = & f & \text{in} \quad \Omega, \\ u & = & 0 & \text{on} \quad \Gamma_D, \\ \partial_n u & = & 0 & \text{on} \quad \Gamma_N, \end{array} \right. \tag{2}$$

where n is the unit outwards normal vector to $\partial\Omega$, and ∂_n stands for the normal derivative on $\partial\Omega$. In addition, let us consider the energy functional depending on the solution u to (2) :

$$E(\Omega, u) \ := \ \frac{1}{2}\int_\Omega \left(|\nabla u|^2 + u^2\right) dx - \int_\Omega f u\, dx = -\frac{1}{2}\int_\Omega \left(|\nabla u|^2 + u^2\right) dx = -\frac{1}{2}\int_\Omega f u\, dx, \tag{3}$$

and let us introduce the regularized shape functional

$$J(\Omega) := E(\Omega, u) + \lambda A(\Omega) - \mu P_c(\Omega)^2, \tag{4}$$

with $A(\Omega)$ and $P_c(\Omega)$ defined by

$$A(\Omega) \ := \ |\Omega|, \tag{5}$$

$$P_c(\Omega) \ := \ \max(0, \ell(\partial\Omega) - c). \tag{6}$$

In the above definitions, $|\Omega|$ denotes the Lebesgue measure of Ω in $\mathbb{R}^2$ and $\ell(\partial\Omega)$ is the 1-dimensional measure of $\partial\Omega$. Constants λ and μ are positive and allow us to take into account

the area and perimeter constraints respectively. The constant c is also positive and corresponds to a shifted perimeter functional, i.e. beyond c, the perimeter constraint becomes active.

For any fixed integer $k \geq 1$, let us consider the following shape optimization problem

$$\max\{J(\Omega) : \Omega \in \mathcal{O}_k\}. \tag{7}$$

Since the exterior boundary of Ω is fixed once for all and equals to ∂U, the domains Ω satisfying (7) are actually determined by their moving boundaries Γ_N.

In the following three sections, we perform the mathematical analysis of problem (7). We show that problem (7) is well posed in the sense that there exists an optimal domain, furthermore, the optimal shape can be characterized by appropriate necessary optimality conditions. For a given topology of an optimal domain there are two different sort of optimality conditions. On the moving boundaries, the shape gradients can be evaluated and the optimality conditions say that the optimal value of the cost cannot be improved by admissible boundary variations. On the other hand, the sign of topological derivatives is fixed inside of the geometrical domain, in such a way that any creation of a small hole cannot improve the value of the cost. The second condition is very strong, it seems, therefore it is a very difficult task to find an optimal domain which satisfies such a condition.

Actually, we study the existence of an optimal domain in section 3, and then the shape sensitivity in section 4, the topological derivatives of the functional J are obtained in section 5. The construction of a level set representation is based on the shape derivatives of J, as it is described in section 6. This formulation provides a practical way to increase the values of the shape functional J. The appearance of new holes is not possible with the only use of the level set method based on the shape derivatives. Therefore, an application of topological derivative allows us to create new holes in order to increase the values of J.

3. Existence of an optimal domain

It can be showed that there exists a domain Ω, solution of (7). We make use of a result from Bucur and Varchon [3] and [4] for the Neumann boundary conditions on the holes. Similar result for the Dirichlet boundary conditions in two spatial dimensions is given by Sverak [30]. With a few changes in the proof of this result, we can apply the results from [3] and [4] to our problem. It is possible without any additional difficulty since the boundary Γ_D is fixed. Thus, we obtain the following theorem

Theorem 1 *Let $\Omega_i = U \setminus \overline{\omega}_i$ be a sequence of open sets such that the number of connected components of $\overline{\omega}_i$ is uniformly bounded. If $\overline{\omega}_i$ converges in the sense of the Hausdorff metric to $\overline{\omega}$, then the solution u_i of the Neumann problem*

$$\left\{ \begin{array}{rcll} -\Delta u_i + u_i & = & f & \text{in } \Omega_i, \\ u_i & = & 0 & \text{on } \partial U. \\ \partial_n u_i & = & 0 & \text{on } \partial \omega_i. \end{array} \right. \tag{8}$$

converges to the solution u of problem (8) on Ω if and only if $|\Omega_i| \to |\Omega|$. (All functions are implicitely extended to zero by setting $u_i = 0$ in ω_i and $u = 0$ in ω and the convergence takes place in $L^2(U)$).

Now it is possible to prove the existence of an optimal domain.

Theorem 2 *For any $k \geq 0$, Problem (7) admits at least one solution $\Omega \in \mathcal{O}_k$.*

Proof. Let $\{\Omega_i\}$, $i = 0, 1, 2, \cdots$, be a maximizing sequence for Problem (7). There exists a subsequence still denoted by Ω_i such that $\Omega_i \to \Omega$ for $i \to +\infty$, in the sense of Hausdorff metric. In what follows, such a convergence is denoted by $\Omega_i \xrightarrow{H} \Omega$. For the definition of Hausdorff

convergence, see [8].

It is shown in [8] that the number of connected components of Ω^c is bounded and we also have by taking the limit

$$\ell(\partial\Omega) \leq \liminf_i \ell(\partial\Omega_i). \tag{9}$$

Thus $\ell(\partial\Omega) < \infty$ since we maximize $J(\Omega)$ and thus $P_c(\Omega)$ is bounded. Using the notion of density perimeter introduced in [2], it is well known that the Hausdorff convergence of Ω_i to Ω implies convergence in the sense of characteristic functions :

$$\Omega_i \xrightarrow{H} \Omega \Longrightarrow \chi_{\Omega_i} \xrightarrow{L^1(U)} \chi_\Omega. \tag{10}$$

As a consequence, we get for $i \to +\infty$, the convergence of Lebesgue measures

$$|\Omega_i| \to |\Omega|. \tag{11}$$

To conclude, we have to prove the convergence of $E(\Omega_i, u_i) = -\frac{1}{2}\int_{\Omega_i} f u_i$. Moreover, we have

$$\begin{aligned}
\left|\int_{\Omega_i} f u_i - \int_\Omega f u\right| &= \left|\int_U f u_i \chi_{\Omega_i} - \int_U f u \chi_\Omega\right| \\
&= \left|\int_U f u_i (\chi_{\Omega_i} - \chi_\Omega) + \int_U f \chi_\Omega (u_i - u)\right| \\
&\leq \|u_i\|_2 \|f(\chi_{\Omega_i} - \chi_\Omega)\|_2 + \|f\chi_\Omega\|_2 \|u_i - u\|_2,
\end{aligned}$$

where $\|.\|_2$ is the norm in $L^2(U)$. According to Theorem 1, we have

$$\|u_i\|_2 \to \|u\|_2 \qquad \text{and} \qquad \|u_i - u\|_2 \to 0. \tag{12}$$

Furthermore,

$$\|f(\chi_{\Omega_i} - \chi_\Omega)\|_2 \to 0 \tag{13}$$

thanks to the convergence in the sense of characteristic functions of χ_{Ω_i} to χ_Ω. Thus, we get

$$E(\Omega_i) \to E(\Omega). \tag{14}$$

Finally, combining convergences (14), (11) and (9), we obtain the inequality

$$J(\Omega) \geq \limsup_i J(\Omega_i). \tag{15}$$

Thus, Ω is a solution to problem (7). ■

Remark 1 *In order to use the shape derivatives, we need the domains with smooth boundaries. The solutions of* (7) *are not necessarily smooth. From now on, we assume the existence of an optimal domain for* (7) *which in addition, is smooth enough.*

4. Shape derivatives

Level set method requires the knowledge of shape gradients for the functional to be maximized. Let Ω be a sufficiently regular domain. The variational formulation of (2) is given by

$$u \in H^1_{\Gamma_D}(\Omega) : \int_\Omega \langle \nabla u, \nabla w\rangle\, dx + \int_\Omega uw\, dx = \int_\Omega fw\, dx \qquad \forall w \in H^1_{\Gamma_D}(\Omega)\ , \tag{16}$$

where $H^1_{\Gamma_D}(\Omega) = \left\{v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma_D\right\}$.

We describe the construction of regular perurbations of Ω, which is used to obtain the shape gradients for shape functionals [5],[29]. Let ξ be a vector field of class C^k with compact support in U. We put $|\xi| = \|\xi\|_{C^k(U;\mathbb{R}^2)}$. Let us consider the transformation $F_\xi = I + \xi$ and define $\Omega_\xi = F_\xi(\Omega)$. We assume that $|\xi|$ is small enough, so that F_ξ is a C^k-diffeomorphism. As a consequence, there exists a unique solution $u^\xi \in H^1_{\Gamma_D}(\Omega_\xi)$ to the variational equation in variable domain Ω_ξ,

$$\int_{\Omega_\xi} \langle \nabla u^\xi, \nabla v\rangle \, dx + \int_{\Omega_\xi} u^\xi v \, dx = \int_{\Omega_\xi} f v \, dx \qquad \forall v \in H^1_{\Gamma_D}(\Omega_\xi). \tag{17}$$

We are going to show that the energy functional $E(\Omega, u)$ is differentiable with respect to the domain and we compute its shape derivative $dE(\Omega, \xi)$ defined for any direction $\zeta = \xi/|\xi|$ of the unit norm $|\zeta| = 1$ by

$$dE(\Omega, \xi) := \lim_{t\to 0} \frac{E(\Omega_\xi, u^\xi) - E(\Omega, u)}{t} \ ,$$

where $t = |\xi|$, and for the sake of simplicity, in the notation we write ξ instead of ζ.

We need to transform (17) on the fixed domain Ω. To this end, we denote u_ξ the transported function defined by the composition

$$u_\xi = u^\xi \circ F_\xi \in H^1_{\Gamma_D}(\Omega). \tag{18}$$

Using the change of variable in (17), we obtain the variational equation satisfied by u_ξ :

$$\int_\Omega \langle (DF_\xi^T)^{-1}\nabla u_\xi, (DF_\xi^T)^{-1}\nabla w\rangle q_\xi \, dx + \int_\Omega u_\xi w q_\xi \, dx = \int_\Omega f_\xi w q_\xi \, dx \qquad \forall w \in H^1_{\Gamma_D}(\Omega), \tag{19}$$

where $f_\xi = f \circ F_\xi$. In the above formulation, DF_ξ is the Jacobian matrix of the transformation F_ξ and q_ξ stands for the determinant of the Jacobian. More precisely, we have

$$DF_\xi = I + D\xi, \tag{20}$$

$$q_\xi = \det DF_\xi = 1 + \mathrm{div}\xi + \det D\xi. \tag{21}$$

It is shown in [6] that u_ξ admits the following Taylor expansion

$$u_\xi = u + u^1(\xi) + \tilde{u}(\xi), \tag{22}$$

where the material derivative $u^1(\xi)$ is the unique solution of the variational equation

$$\begin{aligned} \int_\Omega \langle \nabla u^1(\xi), \nabla w\rangle dx &= \int_\Omega \langle A(\xi)^{-1})\nabla u, \nabla w\rangle dx + \int_\Omega g(\xi) w \, dx \\ &\quad - \int_\Omega \left(uw \, \mathrm{div}(\xi) + u^1 w \right) \, dx \qquad \forall w \in H^1_{\Gamma_D}(\Omega). \end{aligned} \tag{23}$$

The matrix $A(\xi)$ and the function $g(\xi)$ are given by

$$A(\xi) = D\xi + D\xi^T - (\mathrm{div}\xi) I,$$

$$g(\xi) = \mathrm{div}(f\xi).$$

Expansion (22) holds true with the estimates (see [6])

$$\|u_\xi - u\|_{H^1_{\Gamma_D}(\Omega)} \leq c|\xi|, \tag{24}$$

$$\|\tilde{u}(\xi)\|_{H^1_{\Gamma_D}(\Omega)} = \|u_\xi - u - u^1(\xi)\|_{H^1_{\Gamma_D}(\Omega)} \leq c|\xi|^2. \tag{25}$$

Making use of the change of variables (18) in the expression $E(\Omega_\xi, u^\xi) = -\frac{1}{2}\int_{\Omega_\xi}\left(|\nabla u^\xi|^2 + (u^\xi)^2\right)dx$ together with the estimates (24) and (25), we obtain that E is differentiable with respect to the domain and its first order shape derivative is given by

$$\begin{aligned} dE(\Omega;\xi) &= -\int_\Omega \langle \nabla u, \nabla u^1(\xi)\rangle\, dx + \frac{1}{2}\int_\Omega \langle A(\xi)\nabla u, \nabla u\rangle\, dx \\ &\quad - \int_\Omega u u^1(\xi)\, dx - \frac{1}{2}\int_\Omega u^2 \mathrm{div}(\xi)\, dx. \end{aligned} \tag{26}$$

Now, choosing $w = u$ in the variational identity (23), we obtain

$$\int_\Omega \langle \nabla u, \nabla u^1(\xi)\rangle dx = \int_\Omega \langle A(\xi)\nabla u, \nabla u\rangle dx + \int_\Omega g(\xi) u\, dx - \int_\Omega \left(u^2 \mathrm{div}(\xi) + u^1(\xi) u\right) dx. \tag{27}$$

In view of (27), we can get rid of $u^1(\xi)$ in (26) :

$$dE(\Omega;\xi) = -\frac{1}{2}\int_\Omega \langle A(\xi)\nabla u, \nabla u\rangle\, dx - \int_\Omega g(\xi) u\, dx + \frac{1}{2}\int_\Omega u^2 \mathrm{div}(\xi)\, dx. \tag{28}$$

Starting from this expression, we can obtain a more useful expression for the shape derivative. First of all, we turn to the first integral term in the right hand side of (28). We have

$$\begin{aligned} \frac{1}{2}\int_\Omega \langle A(\xi)\nabla u, \nabla u\rangle\, dx &= \int_\Omega \langle D\xi \nabla u, \nabla u\rangle\, dx - \frac{1}{2}\int_\Omega |\nabla u|^2 \mathrm{div}(\xi)\, dx \\ &= \int_\Omega \langle \nabla(\langle \xi, \nabla u\rangle), \nabla u\rangle\, dx - \int_\Omega \langle D^2 u\, \xi, \nabla u\rangle\, dx - \frac{1}{2}\int_\Omega |\nabla u|^2 \mathrm{div}(\xi)\, dx \\ &= -\int_\Omega \Delta u \langle \xi, \nabla u\rangle\, dx + \int_{\partial\Omega} \langle \xi, \nabla u\rangle \langle \nabla u, n\rangle\, d\sigma - \int_\Omega \langle D^2 u\, \xi, \nabla u\rangle\, dx. \\ &= -\frac{1}{2}\int_\Omega |\nabla u|^2 \mathrm{div}(\xi)\, dx. \end{aligned}$$

Since $-\Delta u = f - u$ in Ω, equation (28) becomes

$$\begin{aligned} dE(\Omega;\xi) &= -\int_\Omega f\langle \xi, \nabla u\rangle\, dx - \int_\Omega \mathrm{div}(f\xi) u\, dx \\ &\quad + \int_\Omega \langle D^2 u\, \xi, \nabla u\rangle\, dx + \frac{1}{2}\int_\Omega |\nabla u|^2 \mathrm{div}(\xi)\, dx \\ &\quad + \int_\Omega u\langle \xi, \nabla u\rangle\, dx + \frac{1}{2}\int_\Omega u^2 \mathrm{div}(\xi)\, dx \\ &\quad - \int_{\partial\Omega} \langle \xi, \nabla u\rangle \langle \nabla u, n\rangle\, d\sigma. \end{aligned}$$

Finally we obtain

$$dE(\Omega;\xi) = \int_\Omega \mathrm{div}\left(\frac{1}{2}|\nabla u|^2 \xi + \frac{1}{2}u^2 \xi - f\xi u\right) dx - \int_{\partial\Omega} \langle \xi, \nabla u\rangle \langle \nabla u, n\rangle\, d\sigma. \tag{29}$$

Since $\langle \nabla u, n\rangle = 0$ on Γ_N and ξ has compact support in U, we have

$$dE(\Omega;\xi) = \int_{\Gamma_N} \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{2}u^2 - fu\right) \langle \xi, n\rangle\, d\sigma. \tag{30}$$

Moreover, the shape derivatives of $A(\Omega)$ and $P_c(\Omega)$ are given by

$$dA(\Omega;\xi) = \int_{\Gamma_N} \langle \xi, n\rangle\, d\sigma, \tag{31}$$

$$dP_c(\Omega;\xi) = \mathbb{1}_{\{\ell(\partial\Omega)=c\}} \max\left(0, \int_{\Gamma_N} \mathcal{H}\langle \xi, n\rangle\, d\sigma\right) + \mathbb{1}_{\{P_c(\Omega)>0\}} \int_{\Gamma_N} \mathcal{H}\langle \xi, n\rangle\, d\sigma, \tag{32}$$

$$dP_c(\Omega;\xi)^2 = 2P_c(\Omega) \int_{\Gamma_N} \mathcal{H}\langle \xi, n\rangle\, d\sigma, \tag{33}$$

where $\mathcal{H}$ is the curvature of Γ_N. Thus, the shape derivative $dJ(\Omega;\xi)$ of $J(\Omega)$ is given by

$$dJ(\Omega;\xi) = \int_{\Gamma_N} \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{2}u^2 - fu + \lambda - 2\mu P_c(\Omega)\mathcal{H} \right) \langle \xi, n \rangle \, d\sigma \tag{34}$$

5. Topological derivative

For the sake of simplicity, we assume in this section that $\Omega = U$ (i.e. $\Gamma_N = \emptyset$). Let us now consider the perforated domain $\Omega_\rho = U \setminus \overline{B}_\rho$ where B_ρ is the ball of radius ρ, centered at a point $x_0 \in U$ and with boundary $\Gamma_\rho = \partial B_\rho$. In order to study the topological derivative of the functional J for the linear problem (2), we need to compute the asymptotic expansion of the energy (see (3))

$$E(\Omega_\rho, u_\rho) = -\frac{1}{2} \int_\Omega \left(|\nabla u_\rho|^2 + u_\rho^2 \right) dx,$$

where u_ρ is the solution of the linear problem

$$\begin{cases} -\Delta u_\rho + u_\rho = f & \text{in } \Omega_\rho, \\ u_\rho = 0 & \text{on } \partial U = \Gamma_D, \\ \partial_n u_\rho = 0 & \text{on } \Gamma_\rho. \end{cases} \tag{35}$$

In order to study the topological derivative, we used the so-called truncated domain technique (see [27], [12]). We only present the main sketch of the method used to compute the asymptotic expansion of J and we refer to the appendix for a complete proof of the results. We turn to the truncated domain technique by considering the domain

$$\Omega_R = U \setminus \overline{B}_R, \tag{36}$$

where B_R is the ball of radius $R > \rho$, centered at x_0. We also define the ring $C(R,\rho)$ such that $\Omega_\rho = \Omega_R \cup \Gamma_R \cup C(R,\rho)$ where Γ_R denotes the boundary of the ball B_R i.e. $\Gamma_R = \partial B_R$. (see Figure 2).

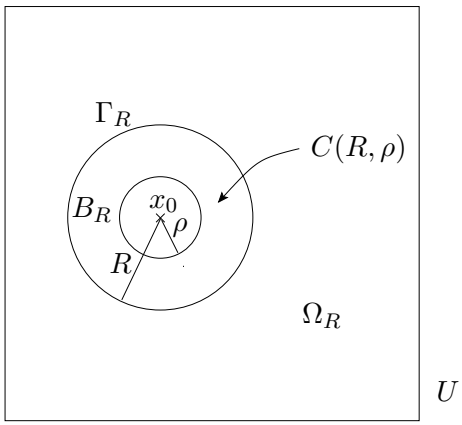

FIG. 2 – The truncated domain technique.

Then we consider the following truncated problem

$$\begin{cases} -\Delta u_\rho^R + u_\rho^R = f & \text{in } \Omega_R, \\ u_\rho^R = 0 & \text{on } \partial U, \\ -\partial_n y_\rho + \partial_n u_\rho^R = A_\rho(u_\rho^R) & \text{on } \Gamma_R. \end{cases} \tag{37}$$

In the above problem, A_ρ is the Stekov-Poincaré operator defined for any $v \in H^{\frac{1}{2}}(\Gamma_R)$ by

$$A_\rho(v) = \partial_n w_\rho, \tag{38}$$

where $w_\rho = w_\rho(v)$ is the unique solution of the problem

$$\left\{\begin{array}{rcll} -\Delta w_\rho + w_\rho & = & 0 & \text{in} \quad C(R,\rho), \\ w_\rho & = & v & \text{on} \quad \Gamma_R, \\ \partial_n w_\rho & = & 0 & \text{on} \quad \Gamma_\rho. \end{array}\right. \tag{39}$$

Finally, the function y_ρ appearing in problem (37) is the solution of the following problem

$$\left\{\begin{array}{rcll} -\Delta y_\rho + y_\rho & = & f_{|C(R,\rho)} & \text{in} \quad C(R,\rho), \\ y_\rho & = & 0 & \text{on} \quad \Gamma_R, \\ \partial_n y_\rho & = & 0 & \text{on} \quad \Gamma_\rho. \end{array}\right. \tag{40}$$

Then, it can be easily shown that

$$u_\rho^R = u_{\rho|\Omega_R} \quad \text{and} \quad u_{\rho|C(R,\rho)} = w_\rho(u_\rho^R) + y_\rho. \tag{41}$$

In order to obtain the topological derivative of J, we have to perform an expansion of the energy functional $E(\Omega_\rho, u_\rho) = -\frac{1}{2}\int_{\Omega_\rho}\left(|\nabla u_\rho|^2 + u_\rho^2\right) dx$ with respect to the radius ρ. Using the domain truncation, we can split the integral in two parts, and we obtain

$$E(\Omega_\rho, u_\rho) = E(\Omega_R, u_\rho^R) - \frac{1}{2}E_\rho^{(1)}(u_\rho^R) + \frac{1}{2}E_\rho^{(2)}(f) \tag{42}$$

where

$$E(\Omega_R, u_\rho^R) = -\frac{1}{2}\int_{\Omega_R}\left(|\nabla u_\rho^R|^2 + (u_\rho^R)^2\right) dx \tag{43}$$

and

$$E_\rho^{(1)}(u_\rho^R) = \int_{C(R,\rho)}\left(|\nabla w_\rho|^2 + w_\rho^2\right) dx \quad \text{with} \quad w_\rho = w_\rho(u_\rho^R), \tag{44}$$

$$E_\rho^{(2)}(f) = -\int_{C(R,\rho)}\left(|\nabla y_\rho|^2 + y_\rho^2\right) dx. \tag{45}$$

Studying problems (37), (39) and (40), we can obtain asymptotic expansion of (43), (44) and (45) respectively which lead to the following expansion for the energy (see the appendix)

$$E(\Omega_\rho, u_\rho) = E(\Omega, u) - \left(\frac{u(x_0)^2}{2} + |\nabla u(x_0)|^2 - f(x_0)u(x_0)\right)\pi\rho^2 + o(\rho^2). \tag{46}$$

Now, using the expansions

$$A(\Omega_\rho) = A(\Omega) - \pi\rho^2, \tag{47}$$

$$P_c(\Omega_\rho)^2 = P_c(\Omega)^2 + 4\pi P_c(\Omega)\rho + o(\rho^2), \tag{48}$$

we obtain the following asymptotic expansion for J :

$$J(\Omega_\rho) = J(\Omega) + h(\rho)\mathcal{T}_\Omega(x_0) + o(h(\rho)), \tag{49}$$

with

$$h(\rho) = \left\{\begin{array}{ll} \pi\rho^2 & \text{if } P_c(\Omega) = 0, \\ \pi\rho & \text{if } P_c(\Omega) > 0. \end{array}\right. \tag{50}$$

The topological derivative $\mathcal{T}_\Omega(x_0)$ of the functional J at point $x_0 \in \Omega$ is given by

$$\begin{array}{l} \bullet \quad \mathcal{T}_\Omega(x_0) = -|\nabla u(x_0)|^2 - \frac{1}{2}u(x_0)^2 + f(x_0)u(x_0) - \lambda, \quad \text{if } P_c(\Omega) = 0, \\ \bullet \quad \mathcal{T}_\Omega(x_0) = -4\mu P_c(\Omega), \quad \text{if } P_c(\Omega) > 0. \end{array} \tag{51}$$

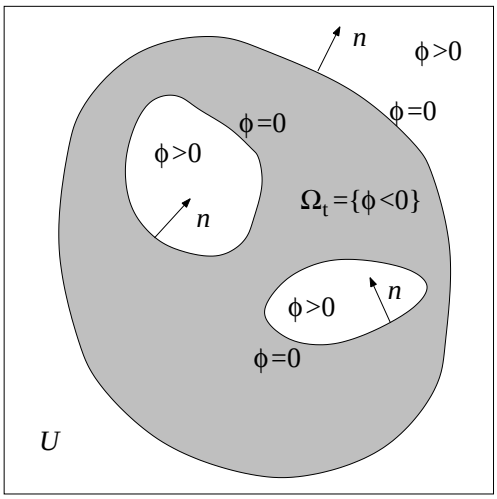

FIG. 3 – The level set representation of the domain.

6. The level set formulation

6.1. The Hamilton-Jacobi equation

In the level set method, a domain and its boundary are represented as level sets of a continuous function ϕ. We refer to [20],[21],[23] for a complete description of the level set formulation of fronts propagating models. We give a brief description of the level set formulation for the evolution of a domain $\Omega \subset U \subset \mathbb{R}^2$ under a given velocity field ξ. Let us consider the domain $\Omega_t = (I + t\xi)(\Omega)$, $t \in \mathbb{R}^+$, with a smooth vector field ξ compactly supported in U. For $t \geq 0$, the domain Ω_t and its boundary are defined by a function $\phi = \phi(x, y, t)$, $(x, y) \in U$, such that

$$\Omega_t = \{(x, y) \in U,\ \phi(x, y, t) < 0\} \quad \text{and} \quad \partial\Omega_t = \{(x, y) \in U,\ \phi(x, y, t) = 0\}. \tag{52}$$

The boundary $\partial\Omega_t$ is the zero level curve of the function $\phi(\cdot, t)$ (see Fig. 3).

We consider the position $(x(t), y(t))$ of a particle on a (given) level curve of $\phi(\cdot, t)$ moving with velocity $\xi = (x'(t), y'(t))$. Then, we have $\phi(x(t), y(t), t) = constant$, for all $t \geq 0$. By differentiating with respect to t, we obtain the following transport equation

$$\phi_t + \xi \cdot \nabla\phi = 0 \quad \text{in } U \times \mathbb{R}^+. \tag{53}$$

The normal unit vectors n to the level sets of ϕ are given by $n = \nabla\phi/|\nabla\phi|$. This leads to the Hamilton-Jacobi equation

$$\phi_t + \xi_n|\nabla\phi| = 0 \quad \text{in } U \times \mathbb{R}^+ \tag{54}$$

where ξ_n is the normal component of the velocity i.e. $\xi_n = \langle \xi, n \rangle$. We also have to choose initial data and boundary conditions with the Hamilton-Jacobi equation (54). The initial data $\phi(x, y, 0) = \phi_0(x, y)$ is chosen as the signed distance function to the initial boundary $\partial\Omega_0 = \partial\Omega$ i.e.

$$\phi_0(x, y) = \pm\ \mathrm{dist}((x, y), \partial\Omega_0) \quad \text{for } (x, y) \in U, \tag{55}$$

with the minus sign (resp. plus sign) if the point x is inside (resp. outside) the initial domain $\Omega_0 = \Omega$. Finally, we choose homogeneous Neumann boundary condition on the boundary ∂U of the whole domain :

$$\partial_n\phi = 0 \quad \text{on} \quad \partial U \times \mathbb{R}^+. \tag{56}$$

6.2. Normal velocity for the level set equation

Recall that the shape derivative $dJ(\Omega;\xi)$ associated to the velocity field ξ is given by (34). We locally (that is under small perturbations of the domain) require that $dJ(\Omega;\xi) > 0$. This leads to the following choice for the normal component $\xi_n = \langle \xi, n\rangle$ of the velocity :

$$\xi_n = \frac{1}{2}|\nabla u|^2 + \frac{1}{2}u^2 - uf + \lambda - 2\mu P_c(\Omega)\mathcal{H} \quad \text{on} \quad \Gamma_N. \tag{57}$$

If the velocity field ξ satisfies (57), we clearly have $dJ(\Omega;\xi) > 0$ and then $J(\Omega_t) > J(\Omega)$ for t small enough.

According to (57), the normal component of the velocity is only imposed along the boundary Γ_N. But in order to solve the Hamilton-Jacobi equation (54), we need a velocity field defined in the whole domain U. We write

$$\xi_n = V_n - 2\mu P_c(\Omega)\mathcal{H} \quad \text{on} \quad \Gamma_N, \tag{58}$$

with

$$V_n = \frac{1}{2}|\nabla u|^2 + \frac{1}{2}u^2 - uf + \lambda \quad \text{on} \quad \Gamma_N. \tag{59}$$

The curvature $\mathcal{H}$ is directly linked to the level set function ϕ by the formula

$$\mathcal{H} = \operatorname{div}\left(\frac{\nabla\phi}{|\nabla\phi|}\right). \tag{60}$$

So, the curvature term is defined in the whole domain U and the only normal velocity part V_n given by (59) has to be extended off the boundary Γ_N. If V_{ext} denotes the extension of V_n to the whole domain U, the Hamilton-Jacobi becomes

$$\phi_t + \left(V_{\text{ext}} - 2\mu P_c(\Omega)\operatorname{div}\left(\frac{\nabla\phi}{|\nabla\phi|}\right)\right)|\nabla\phi| = 0 \quad \text{in } U \times \mathbb{R}^+. \tag{61}$$

The construction of the extension V_{ext} of V_n to the whole domain U is explained in Section 8.

7. The shape optimization algorithm

Now, we describe the general shape optimization algorithm.

First step : initial domain
We start to choose an initial domain Ω^0 and we compute the solution of (2) in Ω^0 by the use of the piecewise linear finite element method. Then, the topological derivative $\mathcal{T}_{\Omega^0}(x)$ is computed for all $x \in \Omega^0$, according to (51).

Second step : topological change by creating a hole
The topological derivative allows us to find the place where a hole should be created in the domain Ω^0 in order to increase the energy functional J. We find the point $x_0 \in \Omega^0$ such that $\mathcal{T}_{\Omega^0}(x_0) = \max_{x\in\Omega^0}\mathcal{T}_{\Omega^0}(x)$. If $\mathcal{T}_{\Omega^0}(x_0) > 0$ then a circular hole ω_ρ of radius $\rho > 0$ and centered at x_0 is created. Then we denote by Ω^0_ρ the domain with the new hole ω_ρ. Homogeneous Neumann condition is imposed on the boundary of the new hole. Remark that the radius of this hole should be as small as possible, depending on the space step of the mesh.

Third step : shape evolution
We turn to the evolution of the domain Ω^0_ρ with the application of the shape derivative in the level set formulation. We have to compute the solution ϕ to the Hamilton-Jacobi equation (61) where the initial ϕ is taken to be the signed distance function to the domain Ω^0_ρ. We perform

the new computation of the solution of (2) in Ω_ρ^0 and then we compute the normal velocity V_n on the internal boundary part Γ_N of $\partial\Omega_\rho^0$ according to (59). The level set equation (61) require to extend the normal velocity V_n to the whole domain U. This is done by solving a transport equation. The next section contains an explaination how to exactly proceed to construct the extended velocity. Only few iterations of the Hamilton-Jacobi equation are performed.

Once we have computed the level set function, we can determine the new domain Ω^1. Then we go back top the first step of the algorithm with Ω^1 in place of Ω^0. We stop when convergence of the domain is reached that is when the geometrical domain does not change anymore.

8. Numerical method for the level set equation

In this section, we present the numerical method used to solve the Hamilton-Jacobi equation (61). We also describe the method used for computing the extension V_{ext} of the normal velocity to the entire domain U.

8.1. Discretization of the level set equation

We choose $U = (0,1) \times (0,1)$ and we define the mesh grid of U by introducing the nodes P_{ij} with coordinates $(i\Delta x, j\Delta y)$. The parameters Δx and Δy are the steps discretization in the x and y directions, respectively. We denote by $t^k = k\Delta t$ the discrete time for $k \in \mathbb{N}$, where Δt is the time step. An approximation $\phi_{ij}^k \simeq \phi(P_{ij}, t^k)$ is computed with a time explicit finite differences scheme due to Osher and Sethian [21],[23],[20]. This scheme is based on an upwind scheme for the first order part $(V_n|\nabla\phi|)$ of the Hamilton-Jacobi equation. For the second order part with the curvature term $(\mathcal{H}|\nabla\phi|)$, centered finite differences are used. More precisely, this scheme reads as

$$\phi_{ij}^{k+1} = \phi_{ij}^k - \Delta t \; g(D_x^-\phi_{ij}^k, D_x^+\phi_{ij}^k, D_y^-\phi_{ij}^k, D_y^+\phi_{ij}^k) \tag{62}$$

where

$$D_x^-\phi_{ij} = \frac{\phi_{ij} - \phi_{i-1,j}}{\Delta x}, \quad D_x^+\phi_{ij} = \frac{\phi_{i+1,j} - \phi_{ij}}{\Delta x} \tag{63}$$

are the backward and forward approximations of the x-derivatives of ϕ at P_{ij}. Similar expressions hold for the approximations D_y^- and D_y^+ of the y-derivatives. The numerical flux is given by

$$g(D_x^-\phi_{ij}, D_x^+\phi_{ij}, D_y^-\phi_{ij}, D_y^+\phi_{ij}) = g_{ij}^{(1)} + g_{ij}^{(2)}. \tag{64}$$

The numerical flux part $g_{ij}^{(1)}$ comes from the discretization of the first order part $V_n|\nabla\phi|$ of the Hamilton-Jacobi equation and is given by

$$g_{ij}^{(1)} \;=\; \max\left(V_{\text{ext}}(P_{ij}), 0\right) \; G^+ + \min\left(V_{\text{ext}}(P_{ij}), 0\right) \; G^- \tag{65}$$

with

$$\begin{aligned} G^+ &= \left[\max(D_x^-\phi_{ij},0)^2 + \min(D_x^+\phi_{ij},0)^2 + \max(D_y^-\phi_{ij},0)^2 + \min(D_y^+\phi_{ij},0)^2\right]^{1/2} \\ G^- &= \left[\min(D_x^-\phi_{ij},0)^2 + \max(D_x^+\phi_{ij},0)^2 + \min(D_y^-\phi_{ij},0)^2 + \max(D_y^+\phi_{ij},0)^2\right]^{1/2} \end{aligned}$$

and $V_{\text{ext}}(P_{ij})$ is the extended normal velocity at point P_{ij} (see the next paragraph for the computation of V_{ext}).

The numerical flux part $g_{ij}^{(2)}$ in (64) comes from the centered finite differences approximation of the second order term of the Hamilton-Jacobi equation i.e.

$$g_{ij}^{(2)} \simeq -2\mu P_c(\Omega)\,\mathcal{H}\,|\nabla\phi|(P_{ij}) = -2\mu P_c(\Omega)\,\text{div}\left(\frac{\nabla\phi}{|\nabla\phi|}\right)\,|\nabla\phi|(P_{ij}). \tag{66}$$

The upwind part of the scheme corresponding to the discretization of the first order term of the Hamilton-Jacobi equation requires the following stability condition of CFL type :

$$(\max_U |V_{\text{ext}}|)\frac{\Delta t}{\min(\Delta x, \Delta y)} \quad \leq \quad \frac{1}{2\sqrt{2}}. \tag{67}$$

Moreover, since we use a centered finite differences scheme for the second order term involving the curvature, the following stability condition of Fourier type has also to be satisfied :

$$4\mu P_c(\Omega)\frac{\Delta t}{\min(\Delta x^2, \Delta y^2)} \quad \leq \quad 1. \tag{68}$$

8.2. Extended normal velocity

As already mentioned, the normal velocity V_n defined by (59) has to be extended to the whole domain U in order to solve the Hamilton-Jacobi equation (61). A natural way to extend V_n off the boundary Γ_N is to seek a function which is constant along the curve normal to Γ_N. This suggests to solve at time t, the following equation for q, up to the stationary state (see [20], [22])

$$q_\tau + S(\phi)\frac{\nabla\phi}{|\nabla\phi|}\cdot\nabla q \quad = \quad 0 \quad \text{in} \quad U\times\mathbb{R}^+ \tag{69}$$

$$q(x,y,0) \quad = \quad p(x,y,t), \quad (x,y)\in U \tag{70}$$

where p equals to V_n given by (59) on the boundary Γ_N and 0 elsewhere. The function S is an approximation of the sign function, defined by

$$S(d) = \frac{d}{\sqrt{d^2 + |\nabla d|^2\varepsilon^2}} \quad \text{with } \varepsilon = \min(\Delta x, \Delta y). \tag{71}$$

Another choices are possible for the approximate sign function (see [22] for details). The extended normal velocity V_{ext} is given by the stationary state reached by the solution q of (69),(70) as the time τ goes to $+\infty$.

At each iteration k of the scheme (62)–(66), we compute the extended normal velocity as the approximate stationary solution of (69),(70). We compute $q_{ij}^m \simeq q(P_{ij}, t^m)$ from the following upwind discretization of (69) :

$$\begin{aligned} q_{ij}^{m+1} = q_{ij}^m - \Delta\tau\Big[\quad & \max(s_{ij}n_{ij}^x, 0)\, D_x^- q_{ij}^m + \min(s_{ij}n_{ij}^x, 0)\, D_x^+ q_{ij}^m \\ & + \max(s_{ij}n_{ij}^y, 0)\, D_y^- q_{ij}^m + \min(s_{ij}n_{ij}^y, 0)\, D_y^+ q_{ij}^m \quad \Big], \end{aligned} \tag{72}$$

where $s_{ij} = S(\phi_{ij}^m)$ and $\Delta\tau$ is a time step such that $t^m = m\Delta\tau$. We use central differences to compute the approximation n_{ij} of the unit normal vector $n = (n^x, n^y) = (\partial_x\phi/|\nabla\phi|,\ \partial_y\phi/|\nabla\phi|)$ at node P_{ij}. The initial value q^0 is equal to V_n on the grid points with a distance to the interface less than $\min(\Delta x, \Delta y)$ and equals zero elsewhere.

8.3. Reinitialization to a distance function

For numerical accuracy, the solution of the level set equation (54) shouldn't be neither too steep nor to flat. This is the case if ϕ is the distance function since we have in that case $|\nabla\phi| = 1$. But even if we start with a distance function for the initial data ϕ_0, the solution ϕ of the level set equation (54) does not remain a distance function. We perform a reinitialization of ϕ at time t by solving the solution $\varphi = \varphi(x, y, \tau)$ of the following equation, up to the stationary state (see [22])

$$\varphi_\tau + S(\phi)(|\nabla\varphi| - 1) \quad = \quad 0 \quad \text{in } U\times\mathbb{R}^+, \tag{73}$$

$$\varphi(x,y,0) \quad = \quad \phi(x,y,t), \quad (x,y)\in U. \tag{74}$$

The function S is the approximate sign function given by (71).

9. Numerical results

In all the numerical tests, we choose $U = (0,1) \times (0,1)$. In the first example (see Figure 4), the topological derivative is used to create holes. In this example, the Hamilton-Jacobi equation is solved on a 51×51 grid. The data are

$$\begin{aligned} &f(x,y) = 10\sin^2(4\pi x), \quad \text{for } (x,y) \in U = (0,1) \times (0,1), \\ &\lambda = 0.5, \ \ \mu = 0, \end{aligned}$$

and the initial domain Ω_0 is the entire domain U i.e. there is no hole in the initial domain. We denote by Ω_1 the optimal domain obtained in this first example. The value of the functional J in Ω_1 is

$$J(\Omega_1) = 0.282319.$$

In the second example (see Figure 5), the topological derivative is not used but only the shape gradient is used for comparison with the previous calculation. In that case, it is therefore necessary to start with a domain with a lot of holes in order to find a domain with a proper topology. In this example, the initial domain is a square with 21 regular holes (see Figure 5) and the data f, λ and μ are the same as in the first example.. In addition, the Hamilton-Jacobi equation is solved on a 101×101 grid. In the second example, the algorithm converges to a local maximum which is lower than the one obtained by using the topological derivative (the first example). Indeed, if we denote by Ω_2 the optimal domain for this second example, we get

$$J(\Omega_2) = 0.2640695 < J(\Omega_1) = 0.282319.$$

Thus Ω_1 allows an increase of 6.5% for the value of the functional J compared to Ω_2. Notice that even without topological derivative, the number of connected components of the complementary set of Ω can increase as can be seen on Figure 5. This is not due to the creation of a hole but due to the splitting of a connected component into two connected components. This is an unusual situation, which should be related to another concept of topological derivative, called the external topological derivative (see [19]).

Additional tests have been performed with $f(x,y) = 10x + y$. In numerical tests depicted on Figure 6 and Figure 7, there is no perimeter constraint ($\mu = 0$). We choose $\lambda = 1$ on Figure 6 and $\lambda = 1.7$ on Figure 7. Small or big oscillations may occur, depending on the value of the weight λ of the volume constraint. On Figure 6 (with $\lambda = 1$), small oscillations occur whereas big oscillations are observed on Figure 7 (with $\lambda = 1.7$). It means that we have no optimal solution for the optimization problem since the perimeter goes to infinity. Finally, Figure 8 shows the smoothing effect of the perimeter constraint for the same source function. In this last example, we have chosen $\lambda = 1.7$ and $\mu = 0.4$.

10. Appendix : The topological derivative with Neumann conditions on the hole

We present the results which are used in Section 5 in order to determine the topological derivative of the energy functional. The asymptotic expansion of the energy is obtained with a domain decomposition technique proposed in [27], [12]. This technique can be described in the following way. The actual domain is divided into two parts $\Omega_\rho = \Omega_R \cup \Gamma_R \cup C(R,\rho)$ (see Figure 2). In the ring $C(R,\rho)$ the singular perturbation of the domain is located, the moving part of its boundary Γ_ρ for $\rho > 0$ is the small parameter. On the other part of its boundary Γ_R the Steklov-Poincaré operator is defined and the asymptotics of the operator are determined in function of the parameter ρ. The second domain Ω_R of the decomposition depends only on the parameter $\rho > 0$ by the nonlocal boundary conditions prescribed in terms of the Steklov-Poincaré operator A_ρ, so we have the regular perturbation of the boundary conditions for the boundary value problem in Ω_R.

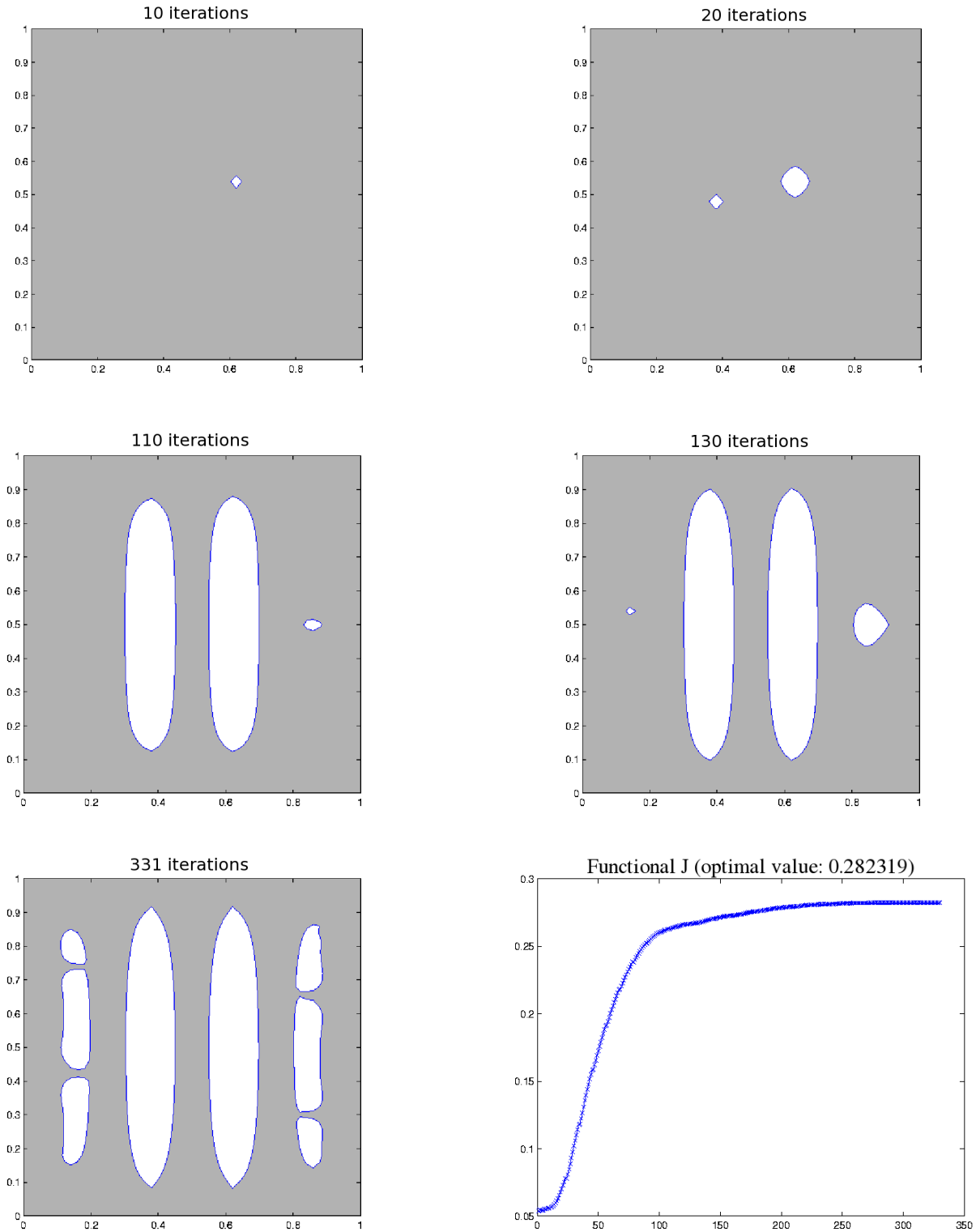

FIG. 4 – Shape optimization with topological derivative. The initial domain is without any holes ($f(x,y) = 10\sin^2(4\pi x),\ \lambda = 0.5,\ \mu = 0$).

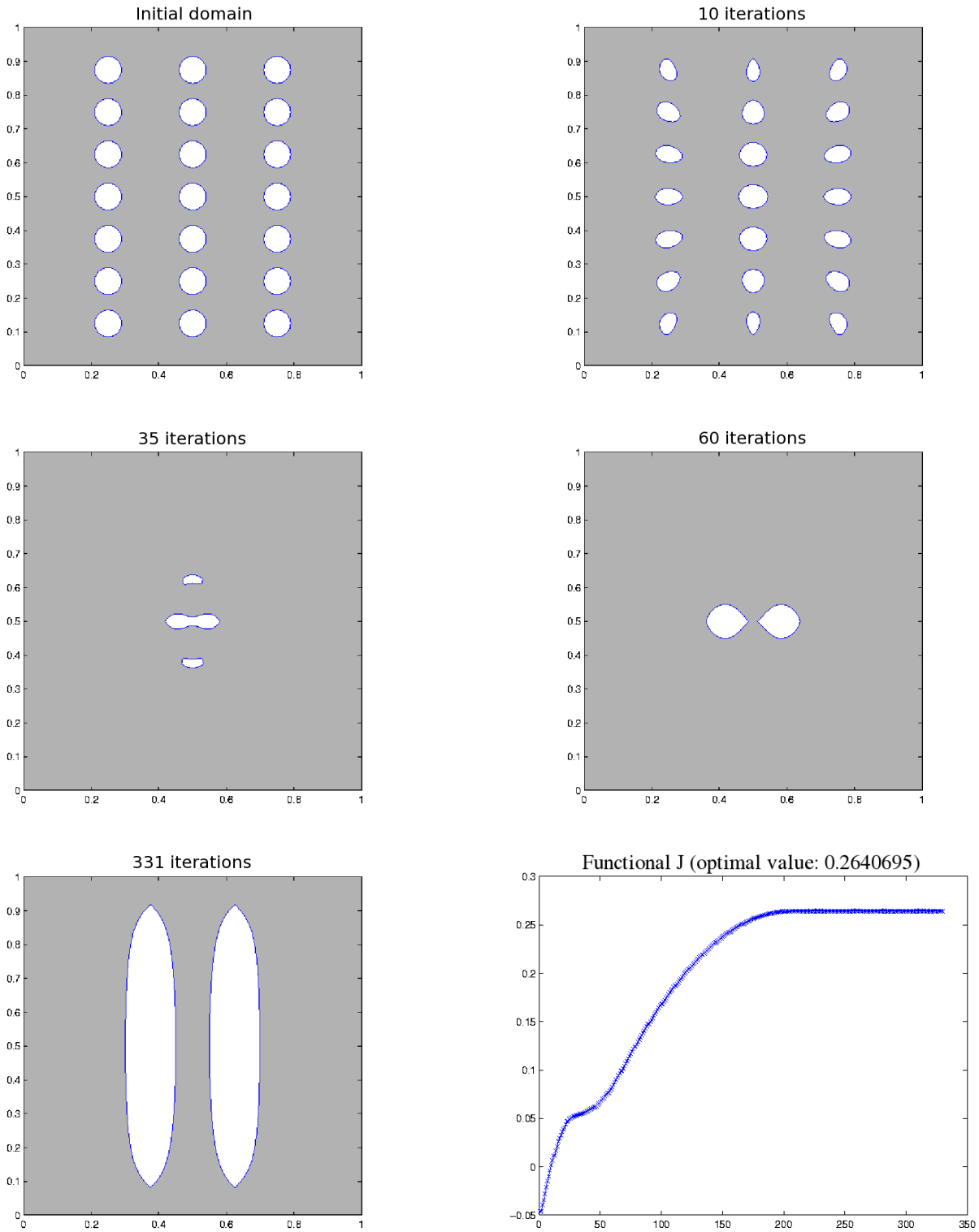

FIG. 5 – Shape optimization without the topological derivative. The initial domain is composed of 21 holes ($f(x,y) = 10\sin^2(4\pi x),\ \lambda = 0.5,\ \mu = 0$).

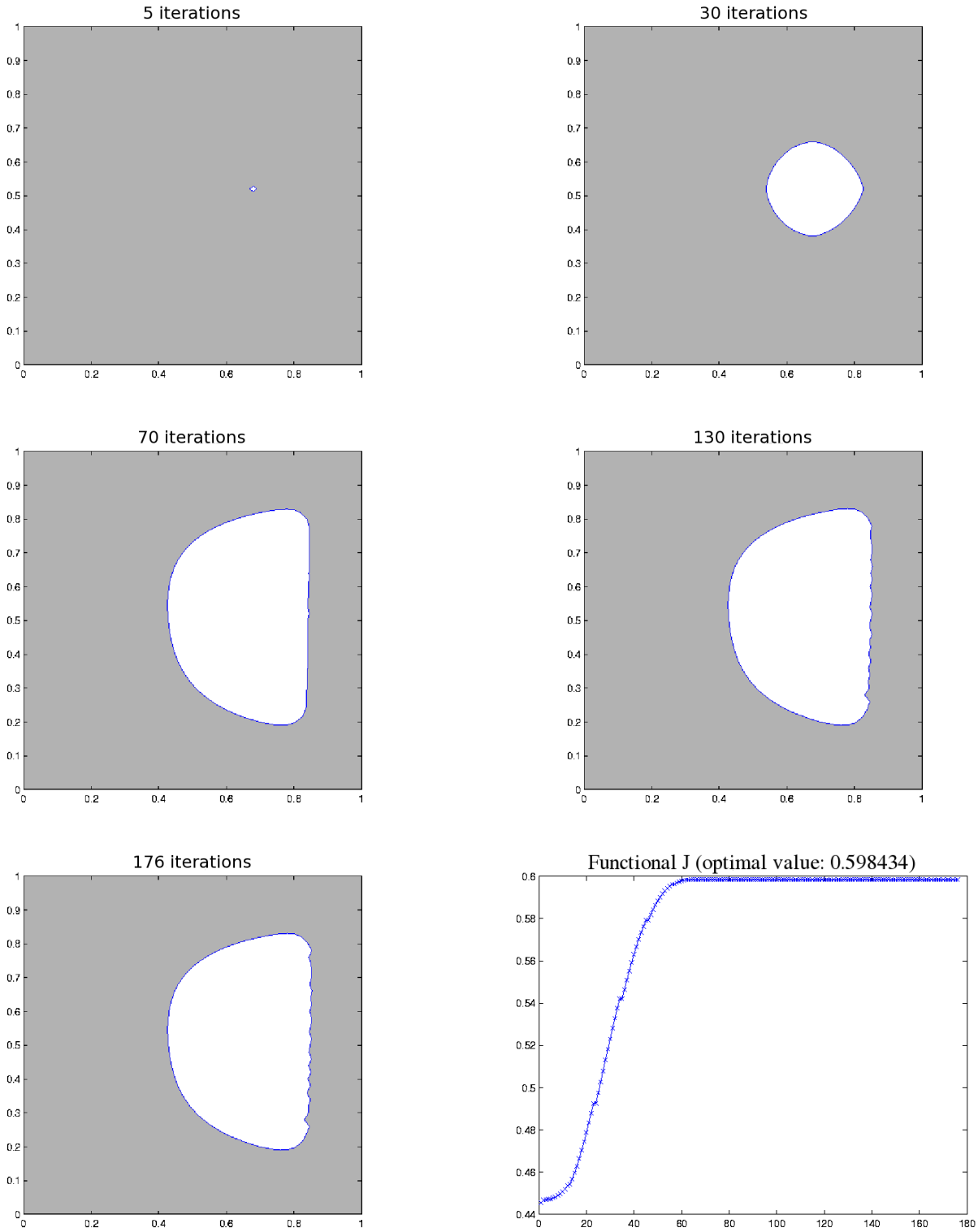

FIG. 6 – Small oscillations without any perimeter constraint ($f(x,y) = 10x + y,\ \lambda = 1,\ \mu = 0$). Optimal value : $J(\Omega) = 0.598434$

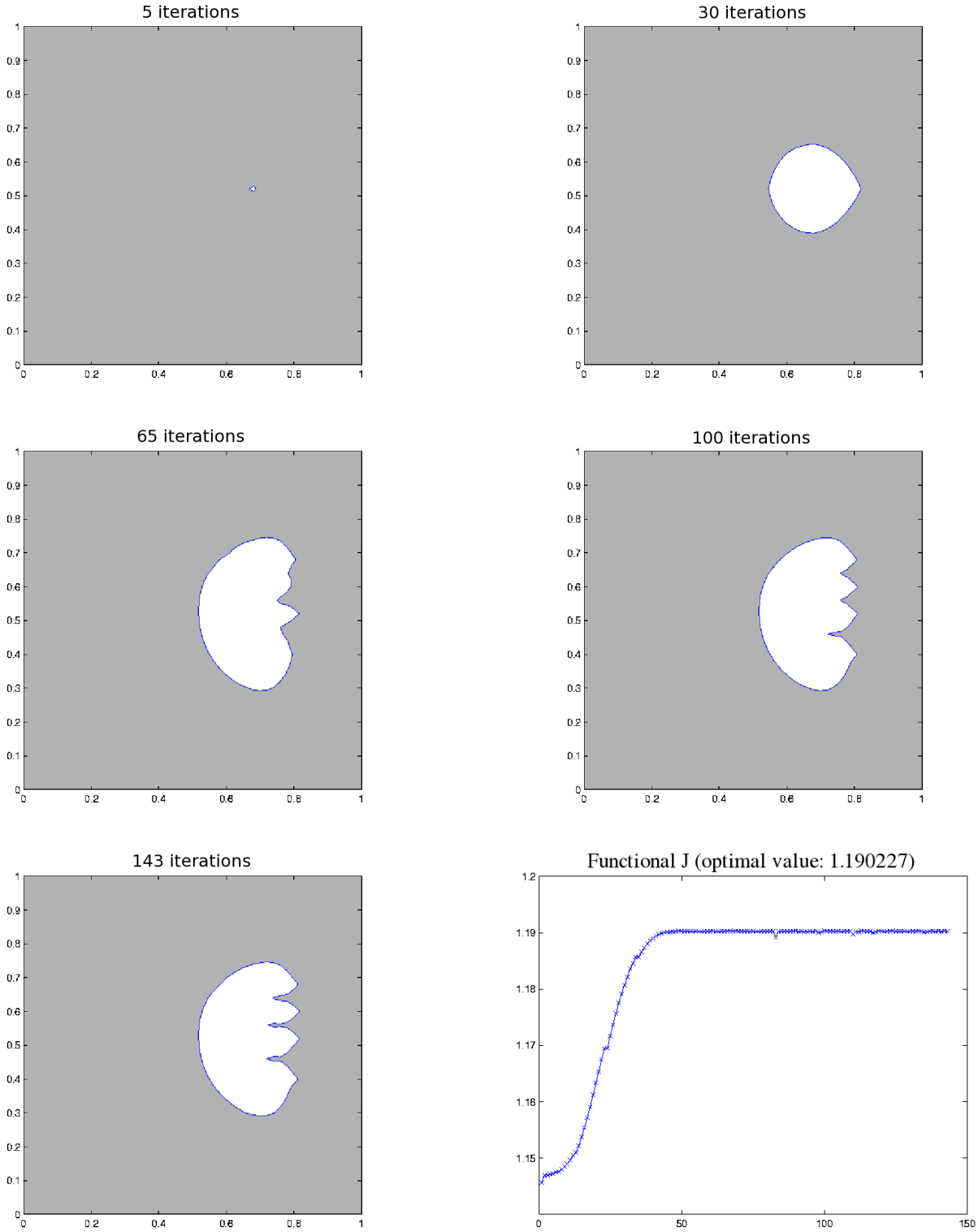

FIG. 7 – Strong oscillations without any perimeter constraint ($f(x,y) = 10x+y,\ \lambda = 1.7,\ \mu = 0$). Optimal value : $J(\Omega) = 1.190227$

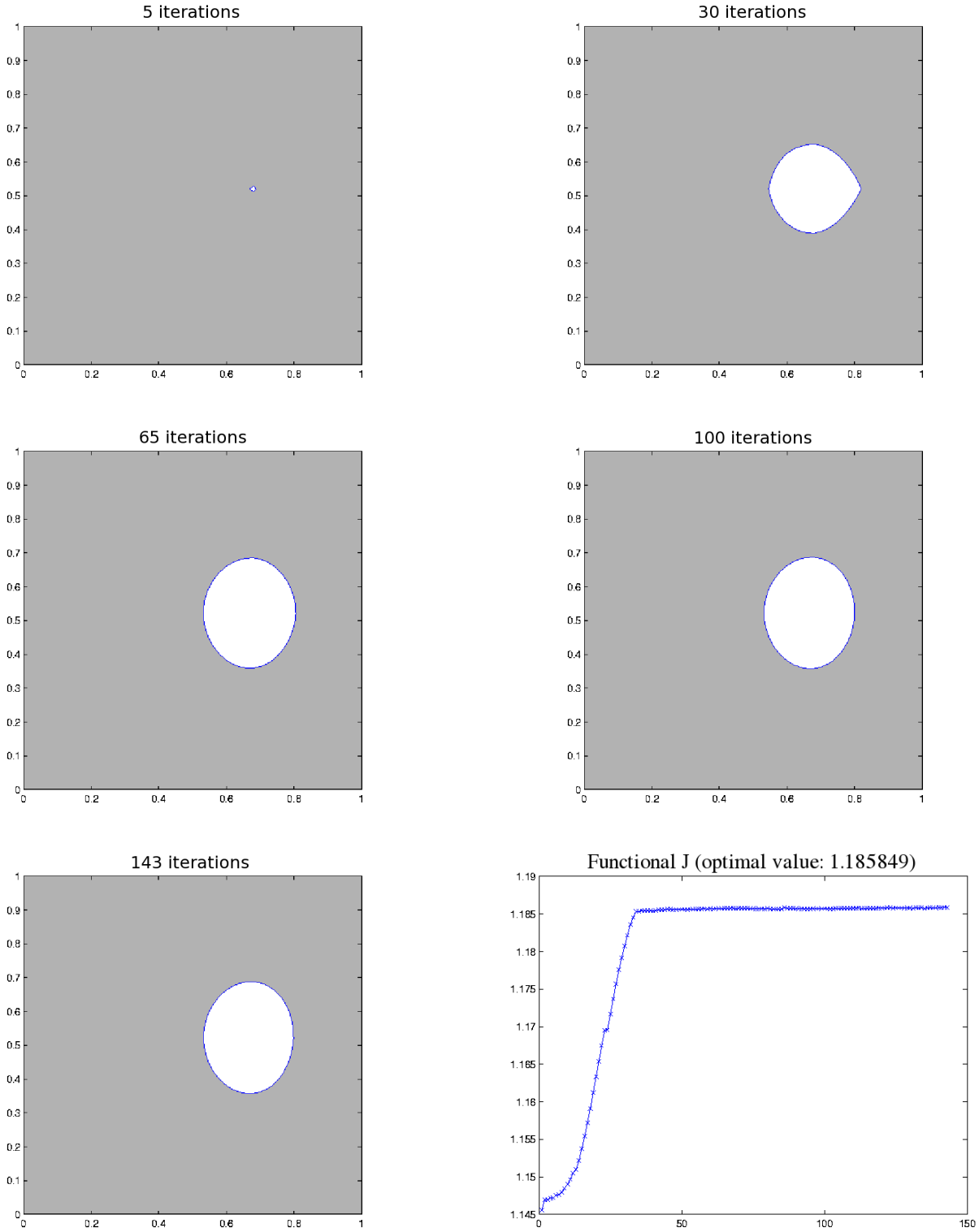

FIG. 8 – Smoothing effect of the perimeter constraint ($f = 10x + y,\ \lambda = 1.7,\ \mu = 0.4$). Optimal value : $J(\Omega) = 1.185849$

Now we give in the next subsections, the asymptotic expansions of the energy terms $E_\rho^{(1)}(v)$, $E_\rho^{(2)}(f)$ and $E(\Omega_\rho, u_\rho)$ appearing in relations (42),(43). For the sake of simplicity, we assume in what follows that $x_0 = 0$.

10.1. Asymptotic expansion of $E_\rho^{(1)}(v)$

For any function v in $H^{\frac{1}{2}}(\Gamma_R)$, let us consider the unique solution $w_\rho = w_\rho(v)$ of the following problem (see (39))

$$\left\{ \begin{array}{rcll} -\Delta w_\rho + w_\rho & = & 0 & \text{in} \quad C(R,\rho), \\ w_\rho & = & v & \text{on} \quad \Gamma_R, \\ \partial_n w_\rho & = & 0 & \text{on} \quad \Gamma_\rho. \end{array} \right. \tag{75}$$

The Steklov-Poincaré operator A_ρ is defined by

$$\begin{array}{rccc} A_\rho : & H^{\frac{1}{2}}(\Gamma_R) & \to & H^{-\frac{1}{2}}(\Gamma_R) \\ & v & \mapsto & \partial_n w_\rho \end{array} \tag{76}$$

We can decompose $v \in H^{\frac{1}{2}}(\Gamma_R)$ in the form of Fourier series with the polar coordinates (r, θ) at the origin :

$$v(\theta) = \frac{1}{2} a_0 + \sum_{k=1}^{\infty} (a_k \sin(k\theta) + b_k \cos(k\theta))$$

and the coefficients satisfy :

$$\sum_{k=1}^{\infty} \sqrt{1+k^2}(a_k^2 + b_k^2) \leq M,$$

where M is a constant depending only on R. This implies two important properties :

$$\sum_{k=1}^{\infty} (a_k^2 + b_k^2) \leq M, \qquad \sum_{k=1}^{\infty} k(a_k^2 + b_k^2) \leq M. \tag{77}$$

We are interested in the asymptotic expansion with respect to ρ of the energy term

$$E_\rho^{(1)}(v) = \int_{C(R,\rho)} \left(|\nabla w_\rho|^2 + w_\rho^2 \right) dx \tag{78}$$

where $w_\rho = w_\rho(v)$ is the solution of (75). We define the energy functional

$$E^{(1)}(v) = \int_{B_R} \left(|\nabla w|^2 + w^2 \right) dx, \tag{79}$$

where w is the solution of

$$\left\{ \begin{array}{rcll} -\Delta w + w & = & 0 & \text{in} \quad B_R, \\ w & = & v & \text{on} \quad \Gamma_R. \end{array} \right. \tag{80}$$

We have the following expansion result for the energy $E_\rho^{(1)}(v)$. For the proof, we refer to [11] or [7].

Theorem 3 *There exists a constant $M > 0$ independant of ρ such that*

$$E_\rho^{(1)}(v) = E^{(1)}(v) - \left(\frac{\pi(a_1^2 + b_1^2)}{2 I_1(R)^2} + \frac{\pi a_0^2}{4 I_0(R)^2} \right) \rho^2 + o(\rho^2),$$

uniformly on bounded subsets of $H^1(\Omega_R)$. The functions I_k for $k \geq 0$, are Bessel functions of first kind defined by $I_k(r) = \displaystyle\sum_{m=0}^{\infty} \frac{\left(\frac{r}{2}\right)^{k+2m}}{m!(k+m)!}$.

10.2. Asymptotic expansion of $E_\rho^{(2)}(f)$

We are now interested in the expansion with respect to ρ of the energy term

$$E_\rho^{(2)}(f) = -\int_{C(R,\rho)} \left(|\nabla y_\rho|^2 + y_\rho^2\right) dx \tag{81}$$

where y_ρ is the solution of the following problem (see (40)) :

$$\left\{ \begin{array}{rcll} -\Delta y_\rho + y_\rho & = & f_{|C(R,\rho)} & \text{in} \quad C(R,\rho) \\ y_\rho & = & 0 & \text{on} \quad \Gamma_R \\ \partial_n y_\rho & = & 0 & \text{on} \quad \Gamma_\rho \end{array} \right. \tag{82}$$

with $f \in C^\infty(\mathbb{R}^2)$. We also need to define the energy term (corresponding to $\rho = 0$ in (81) and (82))

$$E^{(2)}(f) = -\int_{B_R} \left(|\nabla y|^2 + y^2\right) dx, \tag{83}$$

where y is the solution of

$$\left\{ \begin{array}{rcll} -\Delta y + y & = & f_{|B_R} & \text{in} \quad B_R, \\ y & = & 0 & \text{on} \quad \Gamma_R. \end{array} \right. \tag{84}$$

In order to get the asymptotic expansion of $E_\rho^2(f)$, we need to study the function

$$f_{|C(R,\rho)} \mapsto \partial_n y_{\rho|\Gamma_R} = g_\rho.$$

We would like to obtain an expansion of g_ρ with respect to ρ. To this end, we make use of the Fourier expansion of f :

$$f(r,\theta) = \frac{1}{2}\tilde{a}_0(r) + \sum_{k=1}^{\infty} (\tilde{a}_k(r)\sin(k\theta) + \tilde{b}_k(r)\cos(k\theta)).$$

We have the following theorem (we refer to [11] or [7] for the proof) :

Theorem 4 *The function g_ρ admits the expansion*

$$g_\rho = g_0 - \left(\frac{h_0^a(R) - \tilde{a}_0(0)}{4RI_0(R)}\right)\rho^2 - \left(\frac{h_1^a(R)}{2RI_1(R)}\sin\theta + \frac{h_1^b(R)}{2RI_1(R)}\cos\theta\right)\rho^2 + o(\rho^2). \tag{85}$$

where $h_i^a(R)$, $i = 0, 1$ are defined by

$$h_i^a(R) = -\frac{K_i(R)}{I_i(R)}\int_0^R t\tilde{a}_i(t)I_i(t)dt + \int_0^R t\tilde{a}_i(t)K_i(t)dt \tag{86}$$

and $h_1^b(R)$ is obtained from $h_1^a(R)$ by substituing $\tilde{b}_1$ to $\tilde{a}_1$ in (86). In (86), K_i are Bessel functions of second kind [31].

From the previous result, we can deduce the asymptotic expansion for $E_\rho^2(f)$ (see [11],[7]) :

Theorem 5 *There exists a positive constant M independant of ρ such that*

$$E_\rho^{(2)}(f) = E^{(2)}(f) - \frac{\pi h_0^a(R)^2}{4}\rho^2 - \frac{\pi(h_1^a(R)^2 + h_1^b(R)^2)}{2}\rho^2 + o(\rho^2).$$

10.3. Asymptotic expansion of $E(\Omega_\rho, u_\rho)$

Recall that the energy term $E_\rho = E(\Omega_\rho, u_\rho)$ is given by (see (42)) :

$$E_\rho = -\frac{1}{2}\int_{\Omega_R} \left(|\nabla u_\rho^R|^2 + (u_\rho^R)^2\right)\, dx - \frac{1}{2}E_\rho^{(1)}(v) + \frac{1}{2}E_\rho^{(2)}(f),$$

where u_ρ^R is the solution of (37). Using Theorem 3 and Theorem 5, we obtain

$$\begin{aligned} E_\rho - E_0 \;=\; & \int_{\Gamma_R} A_\rho(u_\rho^R)u_0^R\, d\sigma - \int_{\Gamma_R} A_0(u_\rho^R)u_0^R\, d\sigma \\ & -\frac{\pi(h_0^a(R)^2 - 2\tilde{a}_0(0)h_0^a(R))}{8}\rho^2 - \frac{\pi(h_1^a(R)^2 + h_1^b(R)^2)}{4}\rho^2 d\sigma \\ & + \left(\frac{\pi(a_1^2+b_1^2)}{4I_1(R)^2} + \frac{\pi a_0^2}{8I_0(R)^2}\right)\rho^2 + \int_{\Gamma_R} u_0^R \partial_n(y_\rho - y_0)\, d\sigma + o(\rho^2). \end{aligned} \tag{87}$$

It can be proved that

$$u_\rho^R - u_0^R = o(\rho^2), \qquad \partial_n(u_\rho^R - u_0^R) = o(\rho^2), \tag{88}$$

and we deduce that

$$\begin{aligned} \int_{\Gamma_R} A_\rho(u_\rho^R)u_0^R\, d\sigma - \int_{\Gamma_R} A_0(u_\rho^R)u_0^R\, d\sigma \;&=\; \int_{\Gamma_R} (A_\rho - A_0)(u_0^R)u_0^R\, d\sigma + o(\rho^2) \\ &=\; \int_{\Gamma_R} w(u_0^R)\partial_n z_\rho(u_0^R)\, d\sigma + o(\rho^2) \\ &=\; -\frac{\pi a_0^2}{4I_0(R)^2}\rho^2 - \frac{\pi(a_1^2+b_1^2)}{2I_1(R)^2}\rho^2 + o(\rho^2). \end{aligned}$$

Finally, we can calculate the last term of (87), thanks to Theorem 3 :

$$\begin{aligned} \int_{\Gamma_R} u_0^R \partial_n(y_\rho - y_0)\, d\sigma \;&=\; \int_{\Gamma_R} u_0^R(g_\rho - g_0)\, d\sigma \\ &=\; -\pi\left(\frac{a_0(R)h_0^a(R) - \tilde{a}_0(0)a_0(R)}{4I_0(R)} + \frac{a_1 h_1^a(R)}{2I_1(R)}\right)\rho^2 \\ & \quad -\pi\left(\frac{b_1 h_1^b(R)}{2I_1(R)}\right)\rho^2 + o(\rho^2). \end{aligned}$$

With the previous expansions and noticing that $\tilde{a}_0(0) = 2f(0)$, we obtain following expansion result for the energy $E(\Omega_\rho, u_\rho)$:

Theorem 6 *There exists a positive constant M independant of ρ such that*

$$\begin{aligned} E(\Omega_\rho, u_\rho) \;=\; & E(\Omega, u) - \left[\frac{a_0(R)^2}{8I_0(R)^2} + \frac{h_0^a(R)^2}{8} + \frac{a_0(R)h_0^a(R)}{4I_0(R)}\right]\pi\rho^2 \\ & - \left[\frac{a_1(R)^2 + b_1(R)^2}{4I_1(R)^2} + \frac{a_1(R)h_1^a(R)}{2I_1(R)} + \frac{b_1(R)h_1^b(R)}{2I_1(R)}\right]\pi\rho^2 \\ & - \left[\frac{h_1^a(R)^2}{4} + \frac{h_1^b(R)^2}{4} - \frac{f(0)a_0(R)}{2I_0(R)} - \frac{f(0)h_0^a(R)}{2}\right]\pi\rho^2 + o(\rho^2). \end{aligned} \tag{89}$$

The coefficients a_0, a_1 and b_1 are given by

$$a_0(R) = \frac{1}{\pi}\int_0^{2\pi} u(R,\theta)\, d\theta, \quad a_1(R) = \frac{1}{\pi}\int_0^{2\pi} u(R,\theta)\sin\theta\, d\theta, \quad b_1(R) = \frac{1}{\pi}\int_0^{2\pi} u(R,\theta)\cos\theta\, d\theta.$$

The functions $h_i^a(R)$, $i = 0, 1$ are defined in (86).

All the quantities between brackets in the asymptotic development (89) do not depend on R. It can easily be shown that

$$u(0) = \frac{a_0(R)}{2I_0(R)} + \frac{h_0^a(R)}{2}$$

and then

$$\frac{u(0)^2}{2} = \frac{a_0(R)^2}{8I_0(R)^2} + \frac{h_0^a(R)^2}{8} + \frac{a_0(R)h_0^a(R)}{4I_0(R)}.$$

Moreover, we have

$$|\nabla u(0)|^2 = \frac{a_1(R)^2 + b_1(R)^2}{4I_1(R)^2} + \frac{a_1(R)h_1^a(R)}{2I_1(R)} + \frac{b_1(R)h_1^b(R)}{2I_1(R)} + \frac{h_1^a(R)^2}{4} + \frac{h_1^b(R)^2}{4}.$$

Then, we deduce a different expression of the previous asymptotic expansion, which leads actually to the usual expression for the topological derivative

$$E(\Omega_\rho, u_\rho) = E(\Omega, u) + \left[-\frac{u(0)^2}{2} - |\nabla u(0)|^2 + f(0)u(0)\right] \pi\rho^2 + o(\rho^2).$$

Let us mention that for $i = 0, 1$

$$\lim_{R\to 0} h_i^a(R) = 0, \qquad \lim_{R\to 0} h_1^b(R) = 0.$$

Thus, formula (89) gives an expression of the topological derivative which requires the knowledge of u along the boundary Γ_R. This can be interesting from a numerical point of view. In particular, it is possible to calculate $a_1(R)$ and $b_1(R)$ without directly computing the gradient of solution u.

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