Where to place a hole?[1]

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Historically and with respect to increasing order of difficulty as well as generality, structural or topological optimization can be split in three parts.
(i) *Automatic dimensioning of structures* only allowing transformations of the width of different parts of a structure with fixed shape and topology.
(ii) *Shape optimization* allowing shape changes in a fixed topology setting prescribed at the beginning of the process. While this development brought a tremendous improvement over the previous method, in many applications it turned out to be too restrictive.
(iii) *Topological optimization* allowing a more fundamental change of the nature of the structure of interest. It can be seen as the most general shape optimization technique which is currently available. The geometry (of the structure) is considered without any restriction on the connectivity of domains. Compared to other techniques, the flexibility obtained by considering topological changes leads to large improvements in the output of the optimization procedure, for instance in structural mechanics, but also in free boundary problems and various other fields involving shape optimization.

In the early days, many shape optimization models were based on parametric representations of the underlying domains. This caused severe difficulties with respect to topological changes. As a consequence, for practical purposes new theoretical as well as numerical models and techniques needed to be found. In 1985, Murat and Tartar [17] were the first to note that a more generalized notion of domains had to be considered in order to derive appropriate optimality characterizations. The *homogenization theory* represents an important development in this direction. One of its main features consists in considering the domain as a composite material with density ranging from zero to one, rather than defining domains via their characteristic functions, i.e., by a discrete 0-1-valued function. The first numerical application of the homogenization theory was realized by Bendsøe and Kikuchi [5] in 1988. Rather than optimizing the shape by deforming the boundary, the problem was relaxed by considering composite materials defined by a material density distribution and a microstructure, i.e., the shape of the holes on a microscopic scale. This model proved to be very efficient in structural mechanics. Later, various improvements over the original technique were proposed. Among these, we have the so-called SIMP method (SIMP stands for Solid Isotropic Material with Penalization), where the material density is penalized by a power-type law. Despite the fact that the model did not allow a full physical justification, the materials obtained with the SIMP-method were simple and, by avoiding composite materials which were difficult or impossible to manufacture anyway, it solved many practical problems.

The above mentioned topology optimization methods (like the SIMP-method) are very efficient and are still used in many industrial applications; for details we refer to the excellent monograph by Bendsøe and Sigmund [6] covering a number of modelling aspects and numerical techniques. However, their major drawback is due to limitations with respect to possible models and objective functionals.

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For instance, for problems where the boundary is an issue, the homogenization method usually cannot be applied. In order to overcome some of the obstacles, in 1994 Schumacher introduced the so-called *Bubble Method* [9] as a new idea, which keeps the parameterized setting and creates holes in the domain according to some criterion. This idea was later further developed by Sokolowski and Zochowski (1999) [22] as well as Guillaume and Masmoudi (2001) [13] by introducing the notion of a *topological derivative* or *topological asypmtotic*. These latter techniques measure the variation or sensitivity of a shape-dependent cost functional, when a small change in the topology of the underlying domain occurs. This topological change is caused by the creation of a small hole of any shape. In mathematical terms this can be formulated as follows: Let Ω be an open set in $\mathbb{R}^N$, and let $B(x,\varepsilon)$ be the open ball of radius $\varepsilon > 0$ centered at $x \in \Omega$. Define the perforated domain Ω_ε by $\Omega_\varepsilon = \Omega \setminus \overline{B(x,\varepsilon)}$. Whenever the cost functional $J(\Omega)$ is differentiable with respect to the creation of a small hole, e.g., represented by $B(x,\varepsilon)$ for ε sufficiently small, then the expansion

$$J(\Omega_\varepsilon) = J(\Omega) + \rho(\varepsilon)\mathcal{T}(x) + o(\rho(\varepsilon)), \qquad (1)$$

with $\rho(\varepsilon) \to 0$ as $\varepsilon \to 0$, is well-defined. Here, we use $o(s)/s \to 0$ for $s \to 0$. The quantity $\mathcal{T}(x)$ is then called the *topological derivative of J at x*. Note that this topological derivative is a pointwise expression defined at every point of the domain. Therefore it is usually convenient to use and it provides an efficient way to obtain a (topological) descent direction in, e.g., a gradient method. For illustration purposes, as a simple example of a topological derivative we consider here the case when J is the volume of the set Ω. Then one readily finds that $\mathcal{T}(x) = 1$ for all x if $\rho(\varepsilon)$ is chosen as the volume of $B(x,\varepsilon)$. In cases where J involves quantities depending on a partial differential equation (PDE) over the changing domain (such as the solution of the PDE), then the computation of $\mathcal{T}(x)$ usually involves the solution of an adjoint PDE. As an example consider the problem

$$\begin{aligned} &\text{minimize } \frac{1}{2}\int_\Omega (u(x) - u_d(x))^2 dx + \mu \int_\Omega 1\, dx \\ &\text{subject to } -\Delta u = f_\Omega \text{ in } D,\ u = 0 \text{ on } \partial D, \end{aligned}$$

where $u_d \in L^2(D)$ is given, $\mu > 0$ is fixed, $D \subset \mathbb{R}^N$ is sufficiently smooth, and $\Omega \subset D$. Further we have

$$f_\Omega(x) = \begin{cases} 1 & \text{if } x \in \Omega, \\ 0 & \text{else.} \end{cases}$$

Then the topological derivative is given by

$$\mathcal{T}(x) = \begin{cases} -p(x) - \mu & \text{if } x \in \bar{\Omega}, \\ p(x) + \mu & \text{if } x \in D \setminus \bar{\Omega}, \end{cases}$$

where p denotes the adjoint state solving the adjoint equation

$$-\Delta p = u - u_d \text{ in } D,\ p = 0 \text{ on } \partial D.$$

In general, the computation of the topological derivative relies on an asymptotic analysis of the underlying (system of) partial differential equation(s) defined on the perturbed domain. Investigations of these derivatives in various cases (with respect to types of partial differential equations and/or boundary conditions) can be found in the work of Maz'ya and Nazarov on the subject; see [16]. In some cases, the topological derivative can also be retrieved from the classical shape sensitivity calculus, as it is shown in [22] and [19], for instance.

This notion of a topological derivative has already proven to be quite efficient in numerical calculations, and it is also very versatile compared to the homogenization method since the discrete setting is kept for the characteristic function of the sets (i.e.,

the material is not composite). Indeed, the topological derivative can still be used in the context of structural mechanics, but can also be applied in any shape optimization context, especially when the notion of a "material density" becomes irrelevant. Examples of applications of the theory to several fields can be found in [23], [24] for contact and obstacle problems, in [2] and [21] for Navier-Stokes equations, in [3] for electromagnetism, in [11] for linear elastic plate bending problems, and in [4] for time-dependant problems.

Several numerical methods using the topological derivative appeared in the last few years. The first and probably most obvious method consists in using classical parameterizations of the shape as it was the case earlier in shape optimization methods. Then, from time to time in an iterative process, in order to modify the topology holes while be created according to a criterion depending on the topological derivative. For instance, one can remove a small hole in the domain at the point where the topological derivative is most negative. According to the expansion in (1), this results in the steepest decrease in the cost functional. Of course, this set-up requires an according (and possibly numerically expensive) adjustment of the parametrization. Then this new hole can again evolve based on shape sensitivity of the problem. This procedure allows topological changes, but most of the work is done by the shape derivative afterwards.

Since creating a hole wherever the topological derivative is negative should result in a decrease of the functional, one can think of directly removing all the points where this derivative is (sufficiently) negative. Note that such a step is usually not covered by the theory, as simultaneously creating many holes neglects various interdependencies. But in a number of numerical computations this method has proven to be extremely fast, usually catching the appropriate topology within the first one or two iterations. We note, however, that aggressive topology changes may lead to "overshooting" of the optimal domain, and one would need a procedure to recover. In the language of structural optimization this would mean that one has to reinsert material which was removed earlier by the aggressive step.

Recently, the famous "Level-set Method" [20] has been introduced to shape and topology optimization to allow easier and complex topological changes (without the need of expensive re-parameterizations). It relies on implicitly capturing the geometry of interest as the zero-level set of a so-called level set function $\phi : \mathbb{R}^N \times [0, +\infty) \to \mathbb{R}$, $\phi = \phi(x, t)$. Let $\Gamma(t) = \partial\Omega(t) \subset \mathbb{R}^{N-1}$ denote a boundary curve travelling with velocity $F(x(t), t)$ in outward (unit) normal direction. The requirement $\phi(x(t), t) = 0$ for all $x(t) \in \Gamma(t)$ leads to the Hamilton-Jacobi equation

$$\phi_t(x(t), t) - F_e(x(t), t)\|\nabla\phi(x(t), t)\| = 0,$$
$$\phi(\cdot, 0) = \Gamma_0,$$

where F_e is a velocity extending F in a neighborhood of $\Gamma(t)$, and Γ_0 denotes the geometry at $t = 0$. Initially, the method was used without topological derivatives in structural mechanics. In this case, F_e relates to a descent flow based on shape sensitivity (such as the negative shape gradient or a Newton-type flow [14]); see [25] and [8] for an excellent and comprehensive account of shape sensitivity methods. In order to find the correct topology, one had to start with an initial guess containing a large number of holes, which vanished, got merged, or split as the iterations evolved. Such a procedure usually exhibits a significant dependence on the initial guess, i.e., the number, size and shape of the holes. Recently, the topological derivative was introduced successfully to overcome this difficulty; see, e.g.,

[1],[12],[15]. In a phase I–phase II procedure, initially topological sensitivity is used (phase I), which is then followed by shape sensitivity (phase II). As soon as phase II becomes stationary, phase I is restarted. One way of evolving the domain uses the transport equation

$$\phi_t = \delta^{\mathcal{T}},$$

where $\delta\mathcal{T}$ is computed from $\mathcal{T}$ depending on the sign convention for ϕ (e.g., $\phi < 0$ in Ω with $\delta^{\mathcal{T}}(x,t) = -\mathcal{T}(x,t)$ and $\phi > 0$ in $\mathbb{R}^n \setminus \bar{\Omega}$ with $\delta^{\mathcal{T}}(x,t) = \mathcal{T}(x,t)$).

However a lot of questions are still raised by the use of the topological derivative, and a lot of theoretical research is currently performed. For instance, since the above notion of a topological derivative does not cover all possible topological changes, as for instance the creation of a small ligament on the boundary of the set or the splitting of a hole in two holes, currently the so-called *exterior topological derivative* is studied [18]. Another problem is related to the use of the topological derivative on the boundary of a domain. This situation occurs in many numerical applications but has no theoretical foundation. Some results in this direction can be found in [7] and [16]. In order to devise optimality conditions and also a more accurate estimation of the size of the holes, the question of second order information in topology optimization and inverse problems has also been raised recently; see [10]. Further, the concept of creating several holes simultaneously in a domain has also been studied in several papers recently.

In conclusion, the topological derivative appears to be a powerful tool in topological optimization for rapidly finding the appropriate topology and for speeding up shape optimization procedures. But also it may serve as a stand-alone tool. From a theoretical point of view, topological sensitivity analysis is still a very active research field. From a numerical point of view, the method has already proved to be efficient, and has not been fully exploited yet. The numerical methods using topological derivative can be improved by using, e.g., exterior topological derivatives or second order information. Sometimes the topological derivative can be applied in unexpected situations like finding the active or coincidence set $\{u^* = \psi\}$ (see the set in red in Figure 2) in the obstacle problem

$$\text{minimize } \frac{1}{2}\int_\Omega \|\nabla u\|^2 dx - \int_\Omega f\, u\, dx$$
$$\text{subject to } u \le \psi \text{ in } \Omega,$$

where ψ describes the obstacle and the state u represents the displacement of, e.g., a membrane (see Figure 1) on which the force f is exerted.

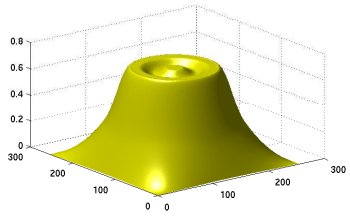

Figure 1: Example of an obstacle problem solved with topological derivative.

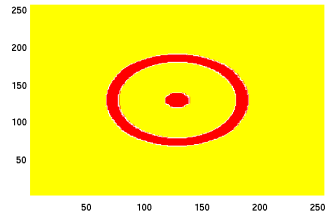

Figure 2: Active set (red) and inactive set (yellow).

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