Topological Optimization with Interfaces

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Abstract Design of architectured materials and structures, whether in nature or in engineering, often relies on forms of optimization. In nature, controlling architecture or spatial heterogeneity is usually adaptive and incremental. Naturally occuring architectured materials exploit heterogeneity with typically graded interfaces, smoothly transitioning across properties and scales in the pursuit of performance and longevity. This chapter explores an engineering tool, topology optimization, that

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is at the frontier of designing architectured materials and structures. Topology optimization offers a mathematical framework to determine the most efficient material layout for prescribed constraints and loading conditions. In engineering, topology optimization is identifying designs with interfaces, materials, manufacturing methods, and functionalities unavailable to the natural world. The particular focus is on the variety of roles that interfaces may play in advancing architectured materials and structures with topology optimization.

1 Introduction

Designing architectured materials and structures introduces a scale for materials organization: this is the "architecture" between the microstructure and macroscopic shape [1–3]. In this approach, "spatial heterogeneity" is controlled such that combinations of materials or of materials and space are arranged in configurations and with connectivities that offer enhanced performance. In this way, interfaces are integral to architectured materials/structures. Interfaces are dynamic, diverse, sometimes dangerous frontiers. The idea of an interface implies the presence of some kind of transition, difference, change, discontinuity, and/or heterogeneity. Within the context of engineering applications, the interfaces of present interest may be mathematical and numerical tools or physically-based constructs. Physically, interfaces occur within and between the primary physical states of matter (solid, liquid, and gas).[1] Mathematically and numerically, interfaces are surfaces, infinitely sharp, that define the boundaries of regions.

Design of architectured materials/structures, whether in nature or in engineering, often relies on forms of optimization. In nature, controlling spatial heterogeneity is usually adaptive and incremental. Naturally occuring architectured materials exploit heterogeneity with typically graded interfaces, smoothly transitioning across properties and scales in the pursuit of performance and longevity. In engineering, topology optimization is identifying architectured designs with interfaces, materials, manufacturing methods, and functionalities unavailable to the natural world. Topology optimization provides a mathematical framework to determine the most efficient material layout for prescribed constraints and loading conditions [4].

This chapter focuses on engineering applications within structural topology optimization and explores the roles that interfaces can play. Within the classification of physical solid or bulk interfaces, several types of interfaces can occur. These include bi-material or hybrid, dissimilar interfaces, heterophase boundaries, localization of defects, grain boundaries, interphases, complexions, interlayers, coatings, and joints. In many of these cases, lattice-parameter changes in the interfacial region, induced by interfacial stresses, may have a pronounced effect on the physical properties and chemical composition at or near the interface [5]. Note that liquid, gas, or mixed , solid/liquid, and liquid/gas interfaces are also of engineering interest but beyond the scope of this chapter. In many structural applications, it is critical to design these material or solid/solid interfaces for system performance. For example, material interfaces often dictate tolerances and processing choices, lifetime and failure characteristics. Recently, the tool of topology optimization has begun to

[1] Plasma and other states of matter that occur under extreme conditions are not considered.

consider more and more numerical and physical roles for interfaces in design. This chapter explores some of these trends and provides perspectives and suggestions for future developments in the context of architectured materials and structures.

2 Structural Optimization

The phrase "structural optimization" is frequently used in engineering fields to describe processes and methodologies which aim to improve some characteristics of a structural part related to its mechanical performance. Historically, mechanical design has been primarily based either on the experience and intuition of designers, or on very simplistic analytical mechanical models. Extensive progress in computation over the last decades has enabled engineers to capitalize on mathematical optimization methods and algorithms to solve increasingly complex structural design problems in an automated manner.

Several categories of structural optimization exist; they depend on the kind of objectives or optimization variables of interest [6–8]. These differences in optimization methods can have dramatic effects on the types of design problems that can be considered and the way that interfaces can be accounted for in the design of architectured materials/structures. The following sections give an overview of the main methods of structural optimization. The focus is on problems of "Topology Optimization" (T.O.), *i.e.* problems where the design variables define the shape and the connectivity of a structure. A general mathematical formulation of a T.O. problem reads:

$$\inf_{\Omega \in \mathscr{U}_{ad}} J(\Omega), \tag{1}$$

where Ω is the domain occupied by the structure, J is the objective function to be minimized and $\mathscr{U}_{ad}$ is a set of admissible shapes constraining the problem and to which Ω shall belong. In general, this problem (eqn. 1) lacks a solution, unless the admissible set, $\mathscr{U}_{ad}$, is adequately constrained.

2.1 Categories of Topology Optimization

A Topology Optimization method can be characterized by two choices: (i) how the structural shape is described and (ii) how the shape evolves during the optimization process. How the shape evolves during the optimization process is directly related to the way a descent direction is calculated, i.e. how a direction that causes a decrease in the objective function to be optimized is found. The majority of T.O. applications use gradient-based methods. Using the calculus of variations, and depending on the nature of the optimization parameters, a descent direction is identified that guarantees the decrease of the objective function, at least for a small change of the design variables. Despite the fact that calculating such a descent direction can be quite cumbersome, very efficient methods have been developed (MMA, CONLIN, MFD, SQP, etc.) that allow one to quickly identify an optimal solution, even for problems with a large number of optimization variables.

In terms of how the structural shape is described, the majority of numerical applications of topology optimization in the literature, as well as commercial software codes, are based on what is called a "density approach" to topology optimization.

In these density approaches, the T.O. problem, (eqn. 1), is translated into a problem of finding an optimal density distribution in a design domain, i.e.

$$\inf_{\theta \in \mathscr{U}_{ad}} J(\theta). \tag{2}$$

The first density approaches to appear in the topology optimization literature used homogenization theory [9–15]. The goal of these approaches was to overcome the difficulty of the non-existence of solutions for the general T.O. problem (eqn. 1) by including "composite" materials as admissible solutions. That is, within a design domain, every point in the domain has an assigned density: 0 for material "A", 1 for material "B", and any value between 0 and 1 represents a kind of "composite" or mixture of "A" and "B" at that point. Note that material "A" or "B" may be physical materials or void (empty space).

Following the early work based on homogenization theory, several simplified methods have been proposed in order to force classical "$0-1$" shapes (shapes that include only solid or void) as solutions to the T.O. problem (eqn. 2). The most well-known among the density approaches is the "Solid Isotropic Material with Penalization" or SIMP method [4]. SIMP uses a simple penalization scheme to suppress the formation of intermediate densities (density values between 0 and 1 with little physical meaning). With the advance of additive manufacturing, the motivation for penalizing these intermediate densities is being reevaluated. Multi-material printers continue to be developed with advanced capabilities. For example, one goal is to mix materials like painters mix red and yellow to achieve any desired orange at any point of interest. A great benefit of these density methods is the simplicity of the description and the ease of computing derivatives with respect to the density field. On the other hand, when the exact position of boundaries of or within the structural shape plays an important role in the mechanics or physics of the problem, density methods are not, in general, well-suited.

Alternatively, geometric methods, as the name implies, use a geometric description of the shape, Ω, and constrain the admissible domain, $\mathscr{U}_{ad}$, to ensure the existence of optimal solutions. In the past, geometric methods have mostly been based on mesh deformation. They were often considered inadequate for performing T.O. due to the difficulty of enacting topological changes while moving the mesh. Recently, the use of level-set methods [16] for T.O. [17–19] made it possible to preserve a geometric description of the shape while perform topological changes in a simplified way. In addition to level-set approaches, advanced mesh deformation methods have also been developed [20] that handle topological changes with mesh evolution. Levelset methods for T.O. will be described in greater detail in section 2.2.1. Geometric methods are usually more complicated than density methods, but they also offer two major benefits. First, they do not inherently introduce intermediate densities into designs. Intermediate densities have limited physical interpretation and $0-1$ designs are usually preferred. Thus, geometric methods do not require further post-processing penalizations and re-interpretations of the design results like most density methods apply for $0-1$ designs. Second, geometric methods can be

applied in any mechanical framework without the need to modify the mechanics of the problem to accommodate intermediate densities.

Other approaches to T.O. include phase-field, evolutionary, and stochastic methods. The phase-field approach combines characteristics from both density and geometric methods [21, 22]. These methods are particularly suitable for multi-material problems, however optimized solutions depend strongly on the penalization parameters used to obtain $0-1$ solutions (without intermediate densities). In the so-called "evolutionary methods," the update of optimization parameters is based on a heuristic criterion. For structural problems, the heuristic criterion is usually a stress-based criterion. This criterion is used to decide whether to add material, to remove material, or to advect a geometric shape [23, 24]. This process is similar to the way that a tree branch will adapt to changing mechanical loads, slowly adding or removing material [25]. Evolutionary methods are very simple to develop, however they are also only effective for a limited range of problems where a heuristic criterion is relevant and readily formulated. Lastly, stochastic methods are well-known for solving general structural optimization problems, mainly involving integer values. However, they are limited to a small number of optimization parameters and their use in Topology Optimization problems that are representative for engineering applications is impractical [26].

2.2 Topology Optimization for interface problems

The choice of the T.O. method to be used for structural design depends strongly on the complexity and the nature of the problem. For example, simplified density methods perform very well for two-dimensional compliance minimization problems and there is no reason to develop an eloborate geometric method in order to obtain similar results. However, for problems where the position of the structural boundary or the precise definition of shape is important, classical density methods may not be sufficient due to the lack of geometric information. There is no explicit definition of an interface for a shape described via a density field varying continuously between 0 and 1. Instead, for T.O. implementations that penalize intermediate density values, the interface is recognized as a region of rapid density variation from 0 to 1. Despite the recent combination of density methods with projection filters [27, 28] in T.O., the position of the interface cannot be described as accurately as when a geometric method is used. In addition, although geometric methods are more difficult to implement numerically and require more complexity to allow topological changes to occur than density approaches, they also present an inherent benefit when it comes to problems where interfaces are important. Namely, the positions of interfaces or shape boundaries are always explicitly defined. This makes all operations related to the interface or shape boundary significantly easier.

2.2.1 Level-set method for T.O.

Since the first publications on the topic of levelset-based T.O. [17–19], there has been rapid growth in this field that is reflected in the numbers of related publications and industrial projects [29]. The combination of the level-set method with the shape sensitivity approach [18, 30, 31] allows one to obtain a gradient-based

geometric method that easily and elegantly performs topological changes. The following provides a brief description of the main elements of a level-set based T.O. algorithm.

Shape description

Using the level-set method for shape description, the boundary of a domain Ω, denoted $\partial\Omega$, is defined as the zero level-set of an auxiliary function ϕ (see Figure 1). Thus, discretizing the level-set function, ϕ, which is part of a larger working domain, D, and defining ϕ as:

$$\begin{cases} \phi(x) = 0 \leftrightarrow x \in \partial\Omega \cap D, \\ \phi(x) < 0 \leftrightarrow x \in \Omega, \\ \phi(x) > 0 \leftrightarrow x \in \left(D \setminus \overline{\Omega}\right), \end{cases} \tag{3}$$

one ensures an immediate and precise knowledge of the interface or shape boundary. It should be noted that, based on the definition in equation 3, a domain, Ω, can

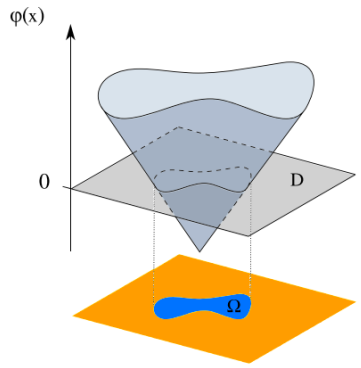

Fig. 1 Level-set based definition of a domain Ω.

be equivalently described by an infinity of level-set functions. A "good" choice of levelset function is one that is smooth enough to guarantee sufficient accuracy for all of the necessary numerical approximations: finding the exterior normal vector, the mean curvature, etc. Such a "good" choice is the **signed-distance function** to the domain, defined as:

$$d_\Omega(x) = \begin{cases} -d(x,\partial\Omega) & \text{if } x \in \Omega, \\ 0 & \text{if } x \in \partial\Omega, \\ d(x,\partial\Omega) & \text{if } x \in \overline{{}^c\Omega}, \end{cases} \tag{4}$$

where $d(x,\partial\Omega)$ denotes the standard Euclidean distance from a point, $x \in \Omega$, to the boundary. Beyond the smoothness of the signed-distance function, its use allows

one to obtain valuable geometric information about the shape in order to define geometric characteristics, like a zone of prescribed thickness.

Another benefit of the level-set framework for T.O. is the ability to capture and describe multiple phases or materials in a natural way [32–34]. By defining n level-set functions in the same design domain and combining their values, one can describe up to $m = 2^n$ different materials (see Figure 2).

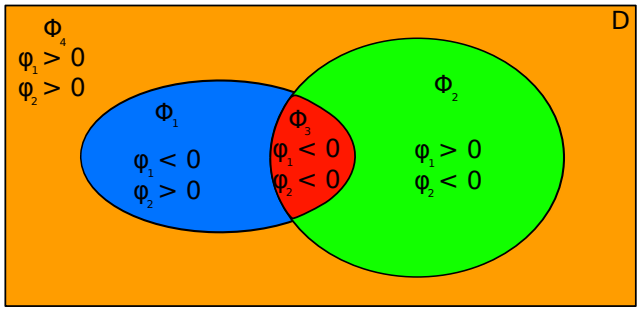

Fig. 2 Multiphase representation in the level-set framework.

Shape derivative

To employ a gradient-based optimization method, one needs to compute a derivative for the functionals contained in the optimization problem with respect to the design variables considered. Using the level-set framework for the description of the shape requires no parameterization of the shape, i.e. the shape is implicitly defined through the values of the discretized level-set function, ϕ, and no design variables need be considered. Instead, the notion of a **shape derivative**, i.e. a derivative of a functional with respect to variations of the shape in a direction $\theta(x)$, which dates back to Hadamard, can be defined as follows [31, 35, 36].

Starting from a domain Ω, one considers perturbations by a smooth enough vector field $\theta(x)$, such that the new domain, Ω_θ, is described by (see Figure 3):

$$\Omega_\theta = \big(Id + \theta\big)\Omega.$$

Then, the shape derivative $J'(\Omega)(\theta)$ of the functional $J(\Omega)$ in a direction $\theta(x)$ is obtained through an asymptotic expansion formula of the type:

$$J\big((Id+\theta)\Omega\big) = J(\Omega) + J'(\Omega)(\theta) + o(\theta) \quad \text{with} \quad \lim_{\theta\to 0} \frac{|o(\theta)|}{\|\theta\|} = 0\,.$$

Once calculated, a descent direction can be found by advecting the shape in the direction $\theta = -tJ'(\Omega)$ for a small enough descent step $t > 0$. For the new shape $\Omega_t = (\mathrm{Id} + t\theta)\,\Omega$, if $V \neq 0$, one can formally write:

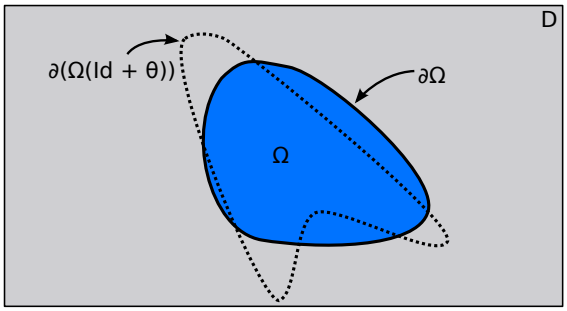

Fig. 3 Perturbation of the domain Ω via a vector field $\theta(x)$.

$$J(\Omega_t) = J(\Omega) - t(J'(\Omega))^2 + \mathscr{O}(t^2) < J(\Omega),$$

which guarantees a descent direction for small positive t.

Shape evolution

During the optimization process the shape is advected with a velocity $V(x)$ obtained from shape differentiation, as presented above. The advection is described in the level-set framework by introducing a pseudo-time, $t \in \mathbb{R}^+$, and solving the well-known Hamilton-Jacobi transport equation:

$$\frac{\partial \phi}{\partial t} + V(x)|\nabla \phi| = 0, \tag{5}$$

using an explicit second order upwind scheme [37], [38].

With this general description of the components of the levelset T.O. method, the following sections focus on how level-set T.O. can account for interfaces from numerical and physical perspectives. In both perspectives, this chapter considers interfaces as either sharp or smooth. Sharp interfaces represent discontinuous jumps. Smooth interfaces represent regions of gradation between distinct regions. Physically and in real materials, examples of both sharp and smooth interfaces can be found. Smooth or graded interfaces are commonly found in naturally occuring architectured materials. Sharp interfaces are representative of the atomically sharp boundaries that can be engineered in modern devices. If one looks at metals at the atomic scale, one can see a physical motivation for both kinds of interface models (sharp or smooth/graded). At an atomic scale it is possible to get a nearly perfectly sharp boundary; this is typically achieved in the semiconductor industry by molecular beam epitaxy. However, in many cases one gets (by design or not) smooth or graded interface zones that are a result of interdiffusion and surface reactions. These graded interface zones can be controlled and tuned by parameters like temperature. All of these types of interfaces serve functions but it is commonly thought that sharp interfaces sacrifice lifetime for performance. Thus, accounting for an engineering interfaces in material/structural design is of great interest.

3 Interfaces as numerical tools in topology optimization

In T.O. one needs to handle criteria that depend on the solution of partial differential equations (PDEs) that represent the physics and mechanics of the problem of interest. These PDEs are defined with respect to a domain, Ω, which is populated by one or more materials and that is a part of a larger working domain, D. The complementary of D, i.e. $D \setminus \Omega$, is filled with a weak material ("ersatz material") representing void or the absence of material. When an interface region between two phases or two materials is present, then the PDE must contain boundary conditions describing compatibility conditions across the interface. In linear elasticity, compatibility conditions typically refer to the displacement fields and the normal component of the stress tensor.

In T.O., treating a sharp interface between different materials or phases is a delicate issue, due to discontinuities in the material properties. This is because discontinuities are not differentiable and the calculation of a shape derivative becomes more tedious. As such, historically, smooth interfaces were initially introduced and used in T.O. as numerical tools to circumvent difficulties related to the differentiation of functionals rather than as models of real interface properties. More specifically, the principle goal of introducing smooth interfaces was to avoid difficulties related to shape differentiation or to avoid limitations of the numerical methods, rather than to represent material realities.

To the best of the authors' knowledge, smooth interfaces in T.O. first appeared in [19] and were followed by a long series of publications that follow this strictly numerical interpretation. In this legacy treatment: (i) mechanical properties are smoothly interpolated across the whole design domain using the level-set function, ϕ, (ii) all of the criteria in the optimization problem are expressed in terms of ϕ, and (iii) classical variational calculus is used to calculate a descent direction, i.e. the derivative of a functional, $J(\phi)$, in a direction, ξ, reads:

$$\left\langle J'(\phi), \xi \right\rangle = \lim_{\delta \to 0} \frac{J(\phi + \delta\xi) - J(\phi)}{\delta},$$

which usually includes much simpler calculations compared to computing a classical shape derivative.

Similar interface modelling was proposed by Allaire et al. in [34] using the signed-distance function (see Figure 4), coupled with a shape derivative. As it is explained in [34], the shape derivative in the multi-material setting contains the jumps of discontinuous stress and strain components across the interface. However, these jumps cannot be computed using Lagrange finite elements on a fixed mesh. Instead of employing techniques that accurately discretize the material interface [20, 39, 40], a remedy to this numerical limitation consists in smoothing the problem using a shape differentiable function (the signed-distance function) and constructing an interpolation scheme that converges to the sharp interface framework when the interpolation width tends to zero.

Beyond smoothing discontinuities or facilitating the derivation, interfaces can also be used numerically to ensure the existence of a minimizer. A minimizer refers

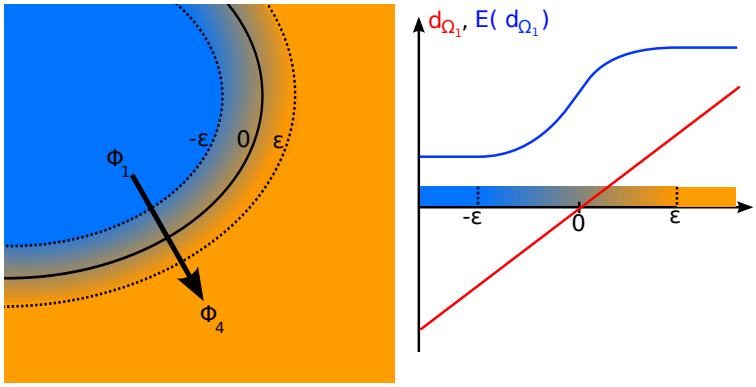

Fig. 4 Interpolation between two phases Φ_1 and Φ_4 using the signed-distance function d_{Ω_1}.

to the case where a sequence of shapes during the optimization process (minimizing sequence) converges to a shape (the minimizer) in $\mathscr{U}_{ad}$. As previously mentioned, the general T.O. problem (eqn. 1) lacks a solution unless the admissible set is adequately constrained. For example, the minimizing sequence may converge to a "composite" design that does not belong to the $\mathscr{U}_{ad}$ that is composed of $0-1$ shapes. Controling the complexity of the shapes in the sequence can be achieved by penalizing the perimeter of the shape [41], choosing smooth vector fields to advect smooth domains [6], or imposing manufacturing constraints like minimum thicknesses [42, 43].

Another approach to stop a minimizing sequence is to add a fictitous interface of constant width. This interface is a numerical tool to control the complexity of design features using a projection scheme [44, 45]. Figure 5 presents a typical example of a bi-material minimizing sequence obtained using a level-set based topology optimization algorithm that imposes an equality volume constraint at each iteration [44, 45]. From left to right, the microstructural features increase in complexity and a highly-interconnected distribution of materials (white and black) is observed. These kinds of minimizing sequences are converging to the theoretical limit in which every point in the domain is occupied by the prescribed volume fraction of materials. For example, if a resource constraint with a volume fraction of 50% of one material (white) and 50% of another material (black) was specified, the optimal solution would be a domain in which every material point is comprised of 50% of each material (the domain would look completely grey). Numerically, the minimizing sequences exhibit features that become vanishingly small while still respecting the required fixed volume fractions of materials at every point in the domain.

Figure 6 illustrates schematically how introducing a fictitous interface of constant width (in grey) can stop a minimizing sequence for the bi-material problem (black and white) with a 50-50 resource constraint. Figure 6 presents, from left to right, an initial design, three intermediate profiles, and the optimal design obtained at convergence with the fictitious interface removed. In this case, the interface is understood as a minimal distance constraint for the members of the projected phase

(in black) [43]. As a result, significant oscillations of the boundary are prevented and the optimization process converges smoothly. The role of the interface here is purely geometric and it is assumed to have the same properties as the weaker material (in white). In this way, an extremely simple, although indirect, way to control manufacturing complexity is achieved.

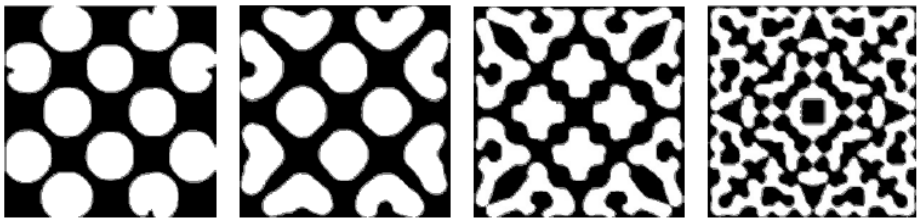

Fig. 5 A minimizing sequence of a bi-material distribution converging weakly to a constant that respects a resource constraint ratio of 50% of each material at each iteration.

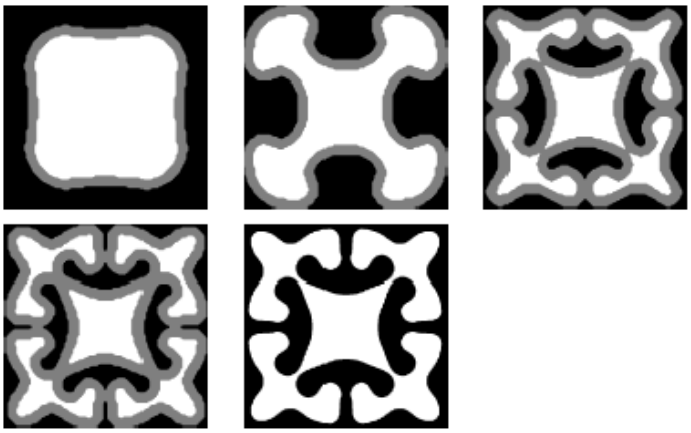

Fig. 6 Using a fictitious interface of constant thickness (in grey) to avoid a minimizing sequence.

4 Considering material interfaces in topology optimization

Beyond numerical reasons, interfaces can be considered in T.O. to represent real material observations. As depicted in Figure 7, the interaction of atoms close to the interface of two phases or materials can result in a region that exhibits properties that are vastly different from the bulk phases or materials. The transition from one phase to another can be monotonic or not, also having a great impact on the optimal configuration.

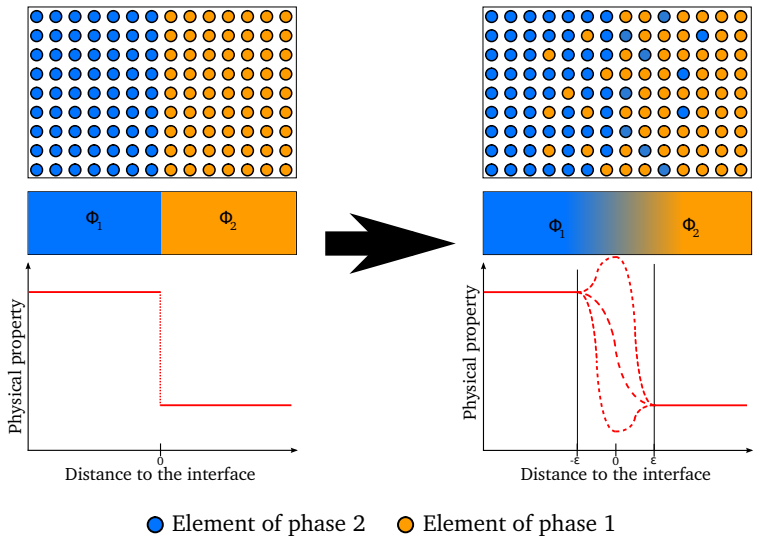

Fig. 7 Left: sharp interface; right: smooth interface with various interpolation schemes.

In order to account for interface effects in T.O., one has to find an appropriate mathematical formulation. The mathematical background presented in [34] for handling smooth interpolation profiles provided the formalism to efficiently treat any kind of regular interpolation scheme. The two key ingredients in this formalism are:

- The use of the signed-distance function in the interface interpolation scheme and
- The use of the co-area formula to obtain a shape derivative.

Using the signed-distance function to interpolate a physical quantity like the Young's modulus, $E(x)$, follows the general form:

$$E(x) = E_0 + h_\varepsilon(d_\Omega)(E_1 - E_0), \text{ where } h_\varepsilon(d_\Omega) = \begin{cases} 0 & \text{if} \quad d_\Omega < -\varepsilon \\ h(d_\Omega) & \text{if} \quad -\varepsilon \leq d_\Omega \leq \varepsilon \\ 1 & \text{if} \quad d_\Omega > \varepsilon, \end{cases} \quad (6)$$

where $h(d_\Omega)$ is a smooth and differentiable function. This formulation requires that the interpolation width (width of the interface zone) remains constant during the optimization process (equal to 2ε). More specifically, if the level-set function, ϕ, is used instead of d_Ω in equation 6, the algorithm could try to enlarge or shrink the interface zone during the shape evolution (see Figure 8) and optimization process in order to improve the objective. This is undesirable for two reasons. First, a great part of the final shape may contain intermediate values for the mechanical properties, eliminating the benefit of using a geometric method. Second, re-initializing the level-set function, ϕ, to the signed-distance function to the domain changes the values of the functionals. As a result, a descent direction is not guaranteed. For more detailed information about this issue, see Allaire *et al.* [34] and Section 3.

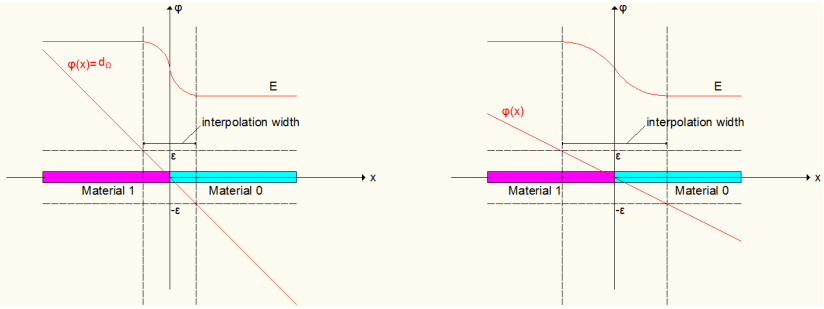

Fig. 8 Interpolation of physical properties using: the signed-distance function d_Ω (left); the level-set function ϕ (right).

The choice of d_Ω in equation 6 comes at the cost of complexity in the shape derivation [34]. This key point has been neglected in previous publications using similar interpolations [19], leading to erroneous formulations. Intuitively, the interface profile considered should have an impact on the advection velocity, and therefore also on the shape derivative. This intuition is substantiated and guaranteed when the correct shape derivation is applied. As explained in [34], using the co-area formula, one can split a volume integral defined in a domain, D, into a surface integral on the internal interface, $\partial\Omega$, and two one-dimensional integrals along the normal lines emerging from every point $y \in \partial\Omega$ (the so-called rays, see Figure 9). Thus, all of the information associated with the interface zone is taken into consideration in the final shape derivative.

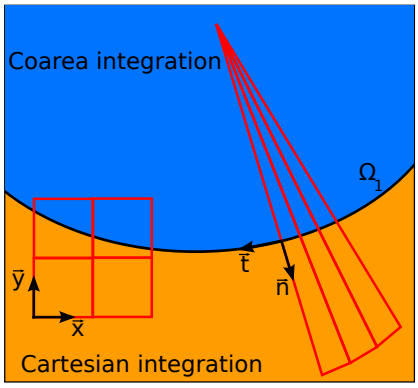

Fig. 9 Rays emerging from the internal intermediate interface, $\partial\Omega_1$.

4.1 Some applications

The influence of incorporating internal material interface zones with distinct material properties in T.O. was first examined in [46] for macroscopic structures. The au-

thors presented the impact of various interface zone interpolation profiles with elastic and thermoelastic example problems. The tendency to augment the total interface perimeter, whenever it is beneficial for the optimization problem, was highlighted and directions for further work to resolve manufacturing issues were proposed.

A similar work in the framework of the SIMP method has also recently appeared in [28] for the design of coated structures. In order to define a notion like an interface using a density approach, the authors deployed a double-projection scheme coupled with a regularization equation. The first projection serves to create a nearly $0-1$ shape. Then, the regularization equation smoothes the density field and the coefficients of the equation are chosen so as to control the regularization width (coating thickness). Lastly, a second projection scheme is applied to obtain the final density distribution.

In this way, two different and powerful approaches for T.O. have recently evolved to address new materials-based design issues. They are now equipped to advance the field of architectured materials and structures by incorporating more interface effects.

In fact, following the work in [46], there is an ongoing effort to understand interface effects in optimal materials design using inverse homogenization [47, 48] (see Figure 10). The research focuses on how interfacial interactions between different phases may affect optimal shapes and material distributions (see Figure 11) in the design of bio-inspired architectured materials.

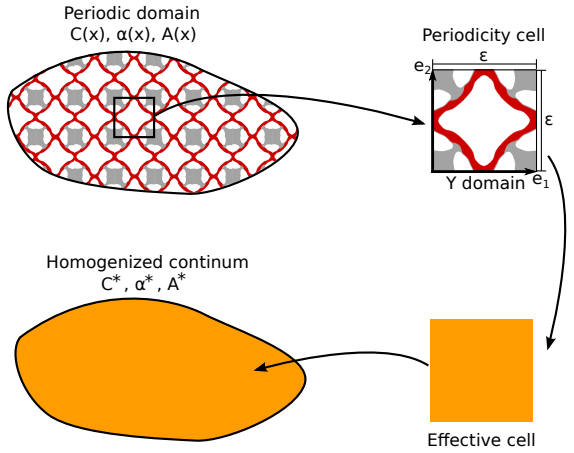

Fig. 10 Inverse homogenization concept: design of a microstructure for target effective properties.

In concert with the advance of T.O. methods, recent progress in additive manufacturing (AM) is expected to significantly broaden the range of T.O. applications. This is due to the extreme design flexibility that additive manufacturing methods afford. The capability to realize increasingly complex geometries allows designers to take full advantage of T.O. and impose fewer manufacturing constraints. As more

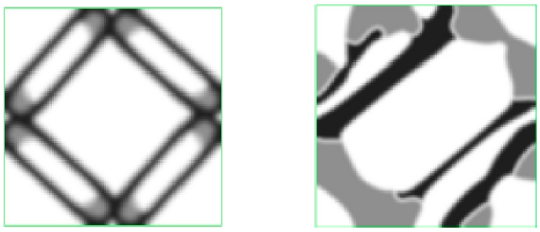

Fig. 11 Optimal microstructure for target elastic and thermoelastic coefficients using a monotone (left) and a non-monotone (right) interpolation scheme.

research is focused on AM techniques and understanding the control of processing features, it is becoming increasingly necessary to tailor T.O. methods to specific AM techniques [49, 50]. For example, several additive manufacturing technologies are known to produce anisotropic properties, or parts with unintended property gradations that are related to the build orientation, build speed, thermal history, and to the in-fill pattern followed during the build process.

One example is that, due to the presence of carbon fibers in some of the printing inks for Fused Deposition Modelling (FDM) printers, the outer structural perimeter or solid/void interfacial layer at the part boundary is characterized by a physical and finite zone where material properties may vary greatly from the interior infill regions. These perimeter zones may have anisotropic properties that result in the stiffness being much greater in one direction relative to the perimeter than another (see Figure 12). The properties of the perimeter zone may play an important role in the overall performance of a printed part, and the anisotropy should be modelled and considered in the optimal design process. This topic is also related to coatings in materials and structures and is the subject of ongoing research.

5 Discussion

The above examples illustrate some of the rich opportunities for including interface effects in topology optimization. In addition to offering a better model of many physical or actual multi-material problems, including interface effects also offers new functionality by leading optimal designs in new directions. Including interface effects may allow optimizers to identify configurations that differ from those identified with classical sharp or monotonic interface modelling. Certainly, for a fixed design domain, these differences become more significant as the presence of the interface zone increases.

One could argue that the area occupied by the interface zone could also be modelled as a third material. The main difference between the interface zone and a third material is that the interface zone, by definition, is always surrounded or in contact with both of the other two materials. Simply introducing a third material does not guarantee or adequately represent this physical feature of interface zones. Nevertheless, this concern is valid and especially relevant when the existence of the interface zone is beneficial for the problem at hand. In this beneficial case, the tendency to promote and create tortuous paths for interface zones puts into question the notion

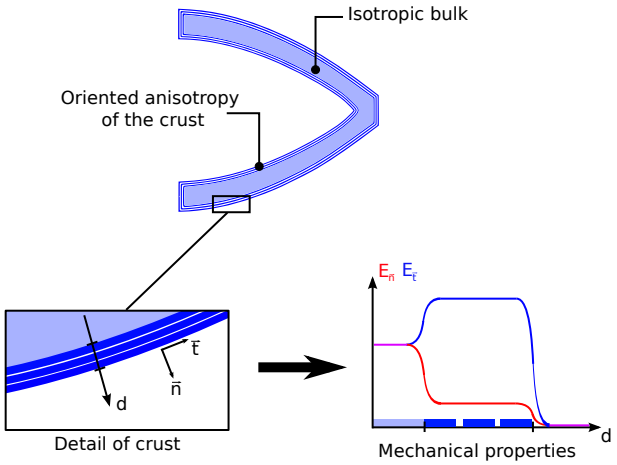

Fig. 12 Schematic of anisotropic perimeter (crust) properties in Fused Deposition Modelling (FDM).

of calling this an interface or interface zone at all. Interfaces, by definition, should also have an associated length scale that is much smaller than the dominant structural feature of the design domain of interest. For example, in Figure 13, one can see how a region of fictitiously high Young's modulus can be assembled by small material islands that approach each other. These islands effectively create an interface network. This artifact is shown in more detail in Figure 14. A non-monotone interface of fixed width is considered between the phase in blue and the one in the grey color. However, since the size of the feature in grey is smaller than the interface width, one can argue that there is no longer an interface between the two phases, but instead a third material with elastic properties defined via the interpolation function.

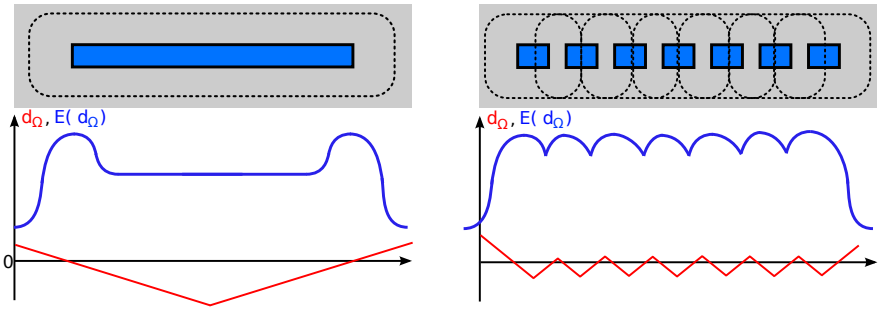

Fig. 13 Interface network resulting in a fictitous overestimation of stiffness.

However, since the position of the interface zone depends on the intermediate interface between the two bulk phases or materials, it is not correct to claim that the

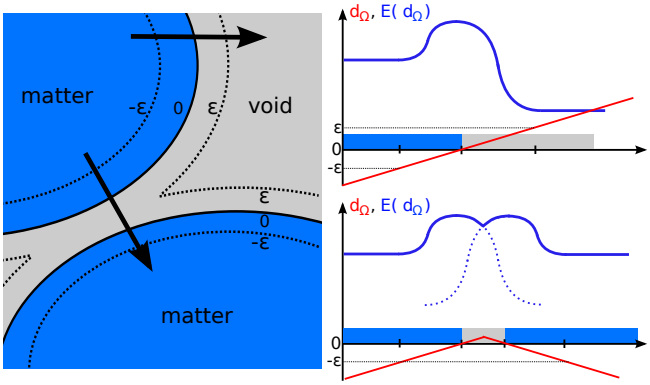

Fig. 14 Another interface network resulting in a fictitous overestimation of stiffness.

interface is simply a third material. Of course, in order to be physically meaningful, geometric constraints are required. Geometric constraint could be applied through a minimum feature size [43] or by using a fictitous interface approach [45]. For example, a projection scheme could be used in order to ensure a minimal distance between structural members and avoid the artifact shown in Figure 13. This could be achieved by offsetting the interpolation scheme (eqn. 6) by a desired distance, d_0 (see Figure 15).

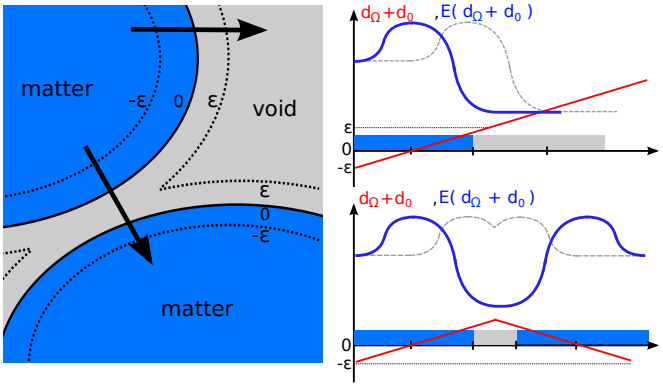

Fig. 15 Imposing a minimal distance d_0 between structural features via a projection method (offsetting the interpolation scheme).

Finally, another topic of interest that is introduced by including interface effects in T.O. is the optimization of the interface property profile itself. There may also be new interface phenomena of interest for T.O. in considering other phases of matter (liquid/gas and solid/liquid interfaces). In all of these cases, instead of imposing prescribed property profiles across interface zone transitions, let the optimization protocol determine optimal property profiles. In theory, it is not difficult to glob-

ally parametrize the interface profile and to proceed with a parametric optimization derivation. One could also consider the interface thickness, as well as the intermediate property value at the center of the interface zone as optimization variables while employing a combined shape and parametric optimization. However, implementation becomes far more complicated when one is interested in locally optimizing the interface profile and a detailed explanation is out of the scope of this chapter.

6 Conclusions

By accounting for interfaces, topology optimization is poised to advance the design and aid the understanding of architectured materials and structures. Whether in nature or in engineering, architecture is allowing designs to capitalize on property differences to extract new or improved performance. Capturing these interface frontiers and transitions across boundaries offers many opportunities and challenges for materials scientists, mathematicians, designers, and engineers. It is suggested that all of these issues are best understood in a holistic context that takes inspiration from nature, manufacturing processes, and performance targets into account.

7 Acknowledgements

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