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TOPOLOGY OPTIMIZATION AND BOUNDARY ELEMENTS: APPLICATION OF TOPOLOGICAL DERIVATIVES TO SOLVE POTENTIAL PROBLEMS IN ORTHOTROPIC MATERIALS

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Abstract: *A numerical approach for topology optimization of orthotropic potential problems using the boundary element methods (BEM) is introduced .The method is based on the evaluation of topological derivative, adopting the total potential energy as the cost function. This procedure is an alternative to the traditional homogenization technique, avoiding solution designs with intermediary material density. In this work, solids with orthotropic behavior are studied under Robin, Neumann and Dirichlet boundary conditions. A well known linear coordinate transformation is used map the original problem and boundary conditions to a new isotropic one, where the optimization procedure is carried out. The optimized solution is then transformed back to the original domain. The proposed approach was found to be particularly suitable to solve this class of problems since in BEM there is no domain mesh to be mapped, reducing significantly the computational cost of the analysis. Some results obtained with this technique are compared and discussed with those available in the literature.*

Keywords: Topology Optimization, Boundary Element Methods, Heat Transfer, Orthotropic Materials, Potential Problems.

1. Introduction

Current modern technologies have produced a great demand increase for non conventional materials. These materials commonly present orthotropic or anisotropic behavior, and special attention must be devoted to the correct characterization of their constitutive properties. As a consequence, the interest in the development of methods and algorithms for optimization of such problems has also increased.

Most of the researches on topology optimization are focused on elasticity problem, while on thermal conduction problems are still very scarce in spite of its importance (Li et al., 1999; Q.Li et al., 2004). Many techniques applied to optimization have been developed in the last decades and are well established in the literature. Certainly one of the most used approaches for topology optimization is the well known homogenization method originally proposed by Bendsøe and Kikuchi (1988). This technique has been successfully employed in many structural problems. Two drawbacks of the homogenization methods are the need to deal with intermediary densities and the possible manifestation of check-board instabilities, which must be controlled. Recently, a new family of methods based on topological derivative (DT) estimates or topological-shape sensibility (Sokolowski and Zochowski, 1997; Feijóo et al. 2003) have been proposed as an alternative to the homogenization methods. The main advantage of DT methods lies in the use of a constant density (avoiding intermediary materiais) and easy implementation. On the other hand, it is rather difficult to be extended to more general cost functions and to include problem dependent restrictions (Garreau et al., 1998; Céa et al.,2000; Sokolowski and Zochowski, 2001; Feijóo, 2002; Novotny et al., 2003). The fact that the BEM does not need domain meshes can be used to reduce significantly the computational cost of iterative processes like optimization. So far, the BEM has been used mostly for shape optimization problems. Marczak (2005) introduced the application of a DT method using the boundary element method (BEM) applied to the topological optimization of linear isotropic potential problems. The objective of the present work is to extend that work to solids with orthotropic or anisotropic behavior. Firstly, the DT formulation focused on the Poisson equation is presented. Next, the basic theory of coordinate transformation method used to solve the anisotropic problem is reviewed. The use of this technique allows the application of DT and the BEM to materials with anisotropic behavior, making this formulation more general, at the cost of very little changes in a standard BEM code. A number of linear heat transfer examples are solved with the proposed formulation and the results are compared with those available in the literature.

2. A view for Topological Derivative

A topological derivative for Poisson Equation is applied in this work. A simple example of applicability consists in a case where a small hole of radius (ε) is open inside the domain. The concept of topological derivative consists in to determine the sensitivity of a given function cost (ψ) when this small hole is increased or decreased. The local value of D_T at a point ($\hat{x}$) inside the domain for this case is evaluated by:

$$\overset{*}{D}_T(\hat{x}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f(\varepsilon)} \tag{1}$$

Where $\psi(\Omega)$ and $\psi(\varepsilon)$ are the cost function evaluated for the original and the perturbed domain, respectively, and f is a regularizing function. With equation (1) was not possible to establish an isomorphism between domains with different topologies. Feijóo et al. (2002) modified the equation introducing a mathematical idea that the creation of hole can be accomplished by single perturbing an existing one whose radius tends to zero. With this new way to state the problem it is possible to establish a mapping between each other (Novotny, 2003).

$$\overset{*}{D}_T(\hat{x}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_{\varepsilon+\delta\varepsilon}) - \psi(\Omega_\varepsilon)}{f(\Omega_{\varepsilon+\delta\varepsilon}) - f(\Omega\varepsilon)} \tag{2}$$

Where δε is a small perturbation on the holes's radius.
In the case of linear heat transfer, the direct problem is stated as:

$$\text{Solve } \{u_\varepsilon \mid -k\Delta u_\varepsilon = b\} \qquad \text{on} \qquad \Omega_\varepsilon \tag{3}$$

$$\text{Subjected to } \begin{cases} u_\varepsilon = \bar{u} & on \quad \Gamma_D \\ k\dfrac{u}{n} = \bar{q} & on \quad \Gamma_N \\ k\dfrac{u_\varepsilon}{n} = h_c\left(u_\varepsilon - u_\infty\right) & on \quad \Gamma_R \end{cases} \tag{4}$$

where:

$$h(\alpha,\beta,\gamma) = \underbrace{\alpha\left(u_\varepsilon - \bar{u}^\varepsilon\right)}_{Dirichlet} + \underbrace{\beta\left(k\frac{\partial u_\varepsilon}{\partial n} + \bar{q}^\varepsilon\right)}_{Neumann} + \underbrace{\gamma\left(k\frac{\partial u_\varepsilon}{\partial n} + h_c^\varepsilon\left(u_\varepsilon - u_\infty^\varepsilon\right)\right)}_{Robin} = 0 \tag{5}$$

is a function which taken into account the type of boundary condition on the holes to be created ($u_\varepsilon, \dfrac{\partial u_\varepsilon}{\partial n}$ are the temperature and flux on the hole boundary, while $u_{\varepsilon\infty}$ and h_c^ε are the hole's internal convection parameters, respectively).

After an intensive analytical work, Feijóo et al. (2002) have developed explicit expressions for DT for problems governed by Eq.(3). These expressions are presented in the next section considering the three classical cases of boundary conditions on the holes.

2.1 Neumann Boundary condition

In this case the eq.(5) is particularized with (α = 0, β =1 , γ = 0) and the D_T is obtained by taking the limit:

$$DT(\ \hat{x}\ ) = -\lim_{\varepsilon \to 0} \frac{1}{2f'(\varepsilon)} \int_{\partial\Omega\varepsilon} \left[k\left(\frac{\partial u_\varepsilon}{\partial t}\right) - k\left(\frac{\partial u_\varepsilon}{\partial n}\right) - 2bu_\varepsilon - \frac{2}{\varepsilon}\bar{q}_\varepsilon u_\varepsilon \right] \ d\Omega\varepsilon \tag{6}$$

And both cases of Newmann boundary conditions must considered:

$$\bar{q}_\varepsilon = \left.\frac{\partial u_\varepsilon}{\partial n}\right|_{\partial\Omega_\varepsilon} = 0 \quad \text{with} \qquad f'(\varepsilon) = -\pi\varepsilon^2 \tag{7}$$

$$\bar{q}_\varepsilon = \left.\frac{\partial u_\varepsilon}{\partial n}\right|_{\partial\Omega_\varepsilon} \neq 0 \quad \text{with} \qquad f'(\varepsilon) = -2\pi\varepsilon \tag{8}$$

For the homogeneous and non-homogeneous cases, respectively. The corresponding expressions for the topological derivatives are (Feijó et al., 2002; Novotny et al., 2003):

$$D_T(\ \hat{x}\ ) = k\nabla u \nabla u - bu \tag{9}$$

$$D_T(\ \hat{x}\ ) = -q_\varepsilon u \tag{10}$$

It is worth to note that both eqs. (9) and (10) are valid for interior and boundary points as well, that is $\hat{x} \in \Omega \cup \Gamma$.

2.2 Dirichlet boundary conditions

The boundary conditions for this case is obtained with (α = 1, β = 0, γ = 0) and the D_T is obtained by taking the limit as :

$$DT(\ \hat{x}\ ) = -\lim_{\varepsilon \to 0} \frac{1}{2f'(\varepsilon)} \int_{\partial\Omega\varepsilon} \left[k\left(\frac{\partial u_\varepsilon}{\partial t}\right)^2 - k\left(\frac{\partial u_\varepsilon}{\partial n}\right)^2 - 2bu_\varepsilon \right] \ d\Omega\varepsilon \tag{11}$$

The conditions:

$$u_\varepsilon = \bar{u}_\varepsilon \qquad\qquad \left.\frac{\partial u_\varepsilon}{\partial t}\right|_{\partial\Omega_\varepsilon} \neq 0$$

are used along with $f'(t) = \dfrac{2\pi}{\ln\varepsilon}$, resulting (Feijó et al. 2002 e Novotny et al. 2003):

$$D_T(\ \hat{x}\ ) = -\frac{1}{2}k\left(u - \bar{u}_\varepsilon\right) \qquad \text{for} \qquad \hat{x} \in \Omega \tag{12}$$

$$D_T(\ \hat{x}\ ) = k\nabla u \nabla u - b\bar{u}_\varepsilon \qquad \text{for} \qquad \hat{x} \in \Gamma \tag{13}$$

Note that D_T is evaluated by different expressions for interior and boundary points, revealing a jump term in its behavior.

2.3 Robin boundary conditions

For this case one has (α = 0, β =0 , γ = 1) e a D_T is obtained by taking the limit:

$$D_T(\ \hat{x}\ ) = -\lim_{\varepsilon \to 0} \frac{1}{2f'(\varepsilon)} \int_{\partial\Omega\varepsilon} \left[k\left(\frac{\partial u_\varepsilon}{\partial t}\right)^2 - k\left(\frac{\partial u_\varepsilon}{\partial n}\right)^2 - 2bu_\varepsilon - \frac{2}{\varepsilon} h_c^\varepsilon \left(u_\varepsilon - 2u_{\varepsilon\infty}\right) \right] \ d\Omega\varepsilon \tag{14}$$

The regularizing the function is found to be $f' = -2\pi\varepsilon$, which results (Feijó et al. 2002 e Novotny et al. 2003):

$$D_T(\hat{x}) = h_c^\varepsilon \left(u_\varepsilon - 2u_{\varepsilon\infty}\right) \quad \text{for} \qquad \hat{x} \in \Omega \cup \Gamma \tag{15}$$

which is valid for any point, as in the Newmann boundary conditions.

3. Basic theory of linear coordinate transformation method

Using conformal mapping techniques, a steady-state orthotropic field problem can be reduced to an isotropic one in the mapped domain. The advantage of this method relies in the fact that the coordinate system of the mapped domain remains orthogonal. The application of numerical methods like the FEM and the BEM to solve steady state field problems governed by the Poisson's equation is well reported in the literature. Poon (1978) investigated the heat conduction problems in layered composites with orthotropic materials. In another publication, Poon et al. (1979) extended the same coordinate transformation for heat conduction for anisotropic media. Shia and Tan (1997) applied the coordinate transformation to map an initial anisotropic to an equivalent isotropic domain. Two examples were solved by using boundary element method and compared with analytical solutions. Hsieh and Ma (2002) introduced in their study a linear coordinate transformation method to solve the heat conduction on a thin layer of anisotropic medium subjected to arbitrary thermal loadings applied inside the domain or on the boundary surfaces. Ma and Chang (2003) studied two-dimensional steady-state thermal conduction problems on anisotropic multi-layered media. They have used the linear coordinate transformation to simplify the governing equation without complicating the boundary and interface conditions. Shiah and Tan (2004) continued their research (Shiah and Tan, 1997) by extending an earlier work to three-dimensional anisotropic field problems.

The differential equation for two dimensional heat conduction in a Cartesian coordinate system (Carslaw and Jaeger, 1959 and Arpaci et al., 1990) is given by:

$$k_{11}\frac{\partial^2 T}{\partial x^2}+2k_{12}\frac{\partial^2 T}{\partial x\partial y}+k_{22}\frac{\partial^2 T}{\partial y^2}=0 \quad (16)$$

where k_{11}, k_{12} and k_{22} are the thermal conductivity coefficients, while T represents the temperature field. The corresponding heat fluxes are expressed as:

$$\begin{aligned} q_x &= -k_{11}\frac{\partial T}{\partial x}-k_{12}\frac{\partial T}{\partial y} \\ q_y &= -k_{12}\frac{\partial T}{\partial x}-k_{22}\frac{\partial T}{\partial y} \end{aligned} \quad (17)$$

A scheme of the mapping is show in figure (1), it is possible to understand that the initial geometry (x) established in an anisotropic media is converted into an equivalent isotropic problem ($\hat{x}$) by using the coordinate transformation.

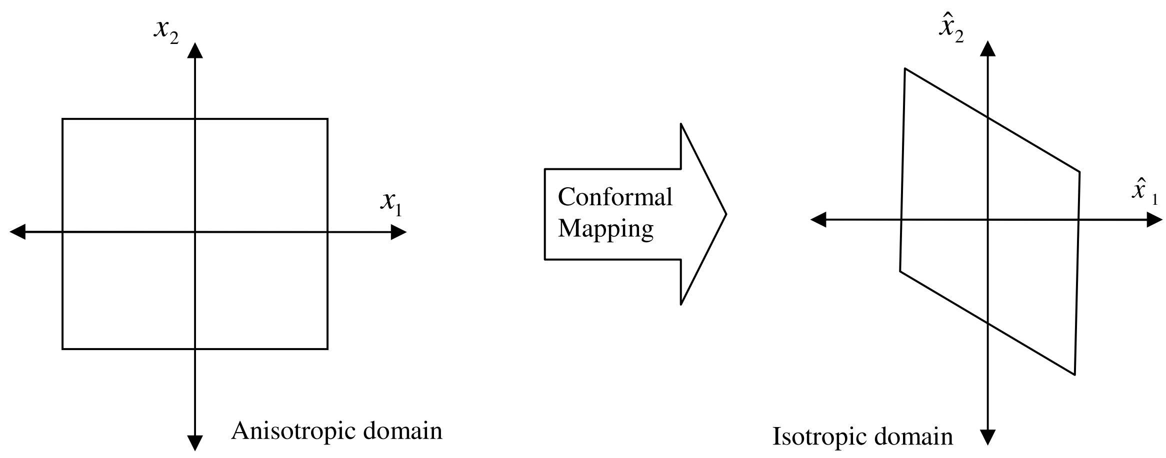


Figure 1. Domain mapping scheme.

Introducing a special linear coordinate transformation to transform the partial differential equation into the Laplace equation as:

$$\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix} = \begin{bmatrix}1 & \alpha\\ 0 & \beta\end{bmatrix} \begin{bmatrix}x\\ y\end{bmatrix} \quad (18)$$

where $\alpha = \frac{-k_{12}}{k_{22}}$, $\beta = \frac{k}{k_{22}}$, $k = \sqrt{k_{11}k_{22} - k_{12}{}^2}$ (19)

Figure 1 illustrates the transformation provided by the mapping of Eq.(18). The originally orthotropic problem on the (x_1, x_2) domain has been converted to an isotropic one defined on the $(\hat{x}_1, \hat{x}_2)$ domain.

Now the governing equation in the transformed domain reads:

$$k\left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2}\right) = 0 \tag{20}$$

where k is the equivalent thermal conductivity given by Eq.(19). It is important to note that the crossed derivative has been eliminated from Eq.(16). Therefore, the transformation (18) resembles the rotation of the constitutive equation to its principal axis. Newmann boundary conditions must be also transformed accordingly:

$$\begin{aligned} q_y &= -k\frac{\partial T}{\partial y} = q_{\hat{y}} \\ q_x &= \beta \quad q_{\hat{x}} - \alpha \quad q_{\hat{y}} \end{aligned} \tag{21}$$

Inverting the Eq.(21), the Newmann boundary conditions are recovered as a function of the original domain boundary conditions.

$$\begin{aligned} q_{\hat{y}} &= q_y \\ q_{\hat{x}} &= \frac{q_x + \alpha \quad q_y}{\beta} \end{aligned} \tag{22}$$

The mapped domain geometry is evaluated through Eq.(18).

4.Numerical Methodology

A heat transfer BEM code developed to isotropic materials was modified to accommodated the linear coordinate transformation (18). This simple approach allows the solution of anisotropic heat transfer problems with very few changes in the original BEM code or further manipulations of the DT formulas. In addition, in the BEM only the boundary nodes have to be transformed, while domain methods like FEM or volume control methods would require the transformation of the domain mesh as well. Another advantage of the BEM is its characteristic good accuracy for boundary variables (both temperature and heat flux) in comparison to other methods, which results in better estimates for DT (Marczak, 2005).

The implemented algorithm encompasses six basic steps:

Step 1: Transform an orthotropic domain into an equivalent isotropic domain by the linear coordinate transformation expressed in equation (18). The heat flux is transformed by equation (21).
Step 2: Solve the problems by the BEM code developed to isotropic materials.
Step 3: Apply the inverse of the mapping domain using equation to the geometry and to the heat flux.
Step 4: The variables are evaluated on a suitable grid of interior points. The points with the lowest values of TD are selected.
Step 5: Holes are created by *punching out* disks of material centered on the previously selected points.
Step 6: Check stopping criteria, rebuilt the mesh, return to step 1.

When the process is halted, the desired topology is expected.

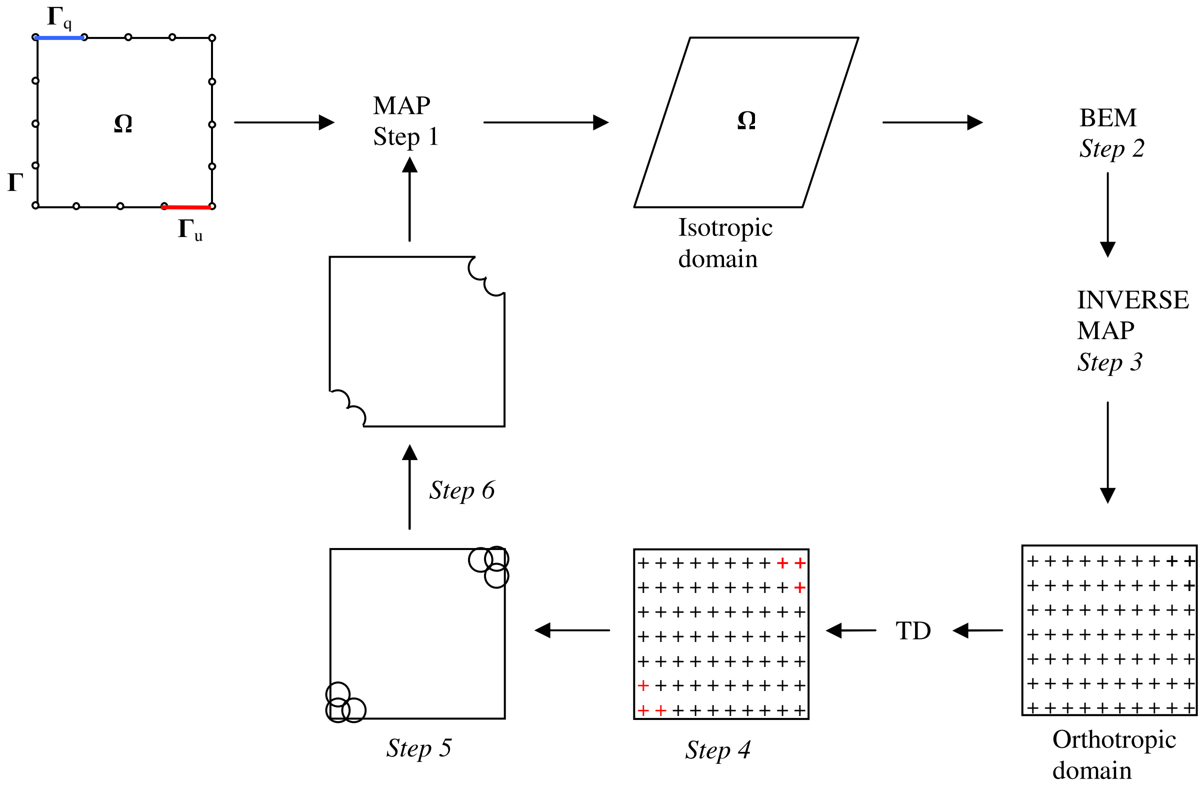


Figure 2. Numerical methodology scheme.

5. Numerical Results

This section presents three examples to demonstrate the application of the proposed method. The main objective of this numerical examples is to extend the topological derivative theory to materials with non isotropic behavior. The benchmarks studied herein are used to verify the material removal history in some simple cases, as well as the final geometries obtained. The results obtained for the first and the second one are compared to those obtained by Novotny et al.(2003) and Marczak (2005, 2006) for isotropic materials. The third example consists of a square domain under high and low temperature boundary conditions where the constitutive relation was varied to simulate all possible behaviors: isotropic, orthotropic and anisotropic.

The material removal history is analyzed and illustrated for each case. The iterative process was stopped when a given amount of material is removed from the original domain, regardless the type of material medium.

In all cases the total potential energy was used as the cost function. A regularly spaced grid of internal points was generated automatically, taking into account the radius of the holes created during each iteration. The radius was taken as a fraction of a reference dimension of the domain ($r = \alpha\ l_{\text{ref}}$). Usually l_{ref} = min(height,width) was adopted. The objective in all cases is to minimize the material volume. The current area of the domain (A_f) was checked at the end of each iteration until a reference value is achieved ($A_f = \beta A_0$, where A_0 represents the initial area). Linear discontinuous boundary elements integrated with 4 Gauss points were used in all cases.

5.1 Example 1 – Asymmetric heat conductor

A square (10×10 mm) domain is subjected to the high (373K) and low (273K) prescribed temperatures on opposite corners. The remaining boundaries (including the cavities that will be open) are insulated. The material to be removed is set with $r = 0.04 l_{ref}$ and the thermal conductivities were defined by $k_x/k_y = 2$. The evolution of the process is shown in Fig. 3. The process was halted when $A_f = 0.8A_0$ was reached. Figure 4 illustrates a comparison between the orthotropic topology obtained with the present approach and the isotropic BEM solution obtained by Marczak (2005) and the FEM solution of Novotny et al. (2003).

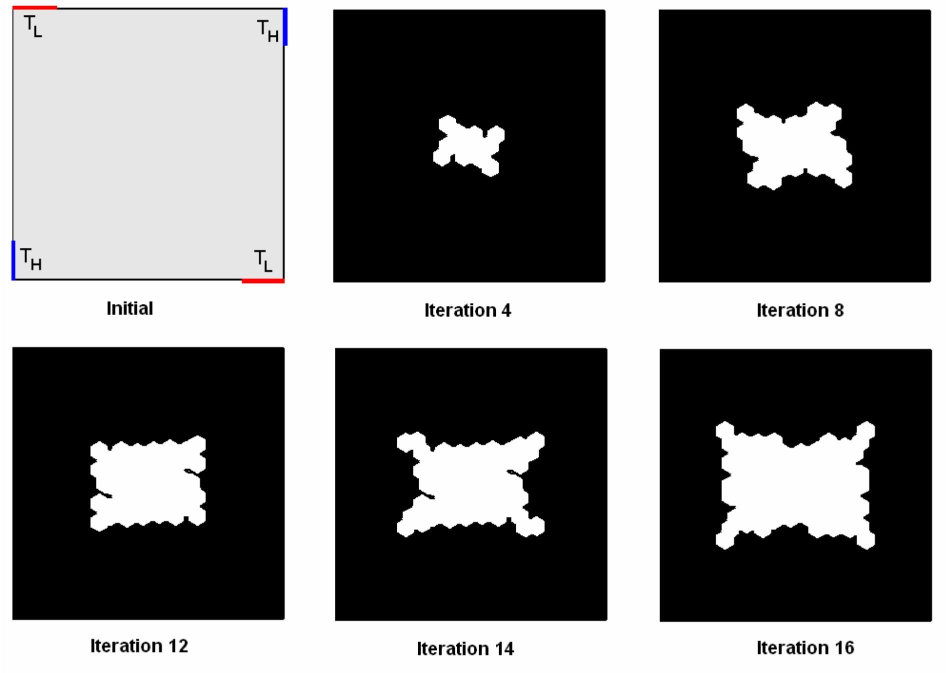
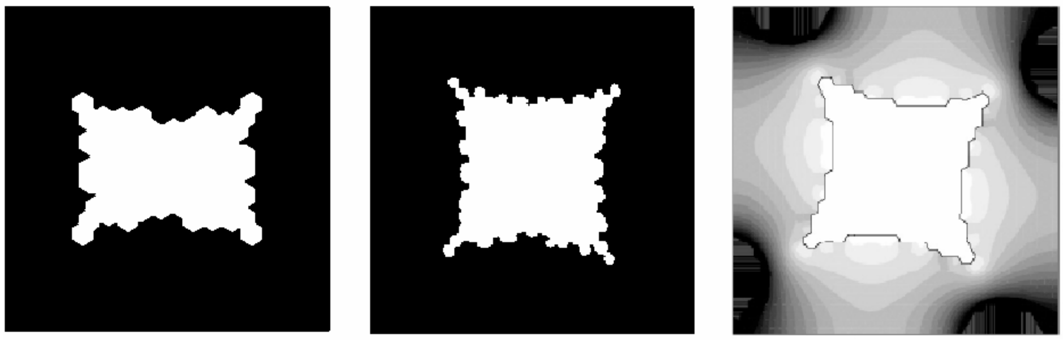


Figure 3. Evolution history to eliminate 20% of material in case 2.

Figure 4 shows how the orthotropic solution differs from the isotropic one. As shown in Fig.8, the algorithm tries to remove more material in the *x* direction, in such a way that the heat flux is more easily transferred between two adjacent corners.



(a) (b) (c)

Figure 4 - Final topologies for the asymmetric conductor: (a) Present result, $k_x/k_y = 2$;
(b) BEM solution for $k_x/k_y = 1$ (Marczak, 2005); (c) FEM solution for $k_x/k_y = 1$ (Novotny et al., 2003).

5.2 Example 2 – Inverted V heat conductor

This example consists in a square domain with high temperature (373 K) prescribed on its lower corners, while a low temperature (273 K) is prescribed at the mid top edge. The remaining boundaries are insulated. The cavities were created with r= $0.04 l_{ref}$ and the process was halted when $A_f = 0.6\ A_0$ is attained. In order to illustrate and compare the final topologies obtained, three variations of the present example are studied as:

Case A: $k_{xx} = 1$; $k_{yy} = 1$
Case B: $k_{xx} = 2$; $k_{yy} = 1$
Case C: $k_{xx} = 3$; $k_{yy} = 1$

Figure 5 shows the results for the isotropic case (case A) wich will be used to compare the final design with the orthotropic cases (cases B and C). Figures 6 and 7 present the optimization evolution for the orthotropic case and their final topology when the stop criteria was achieved. Now, it is possible to compare the three cases. There are visible differences in the material removal evolution for each case, although the final designs are slightly different in this case.

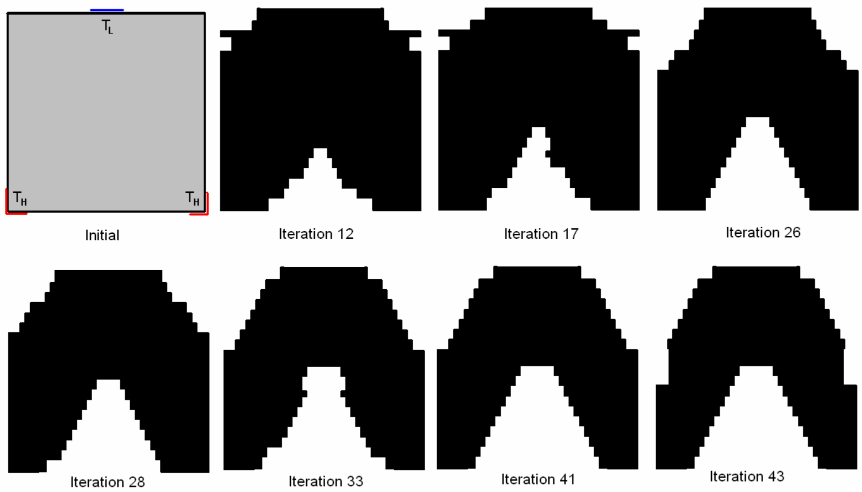


Figure 4. Evolution history for isotropic material – Case A.

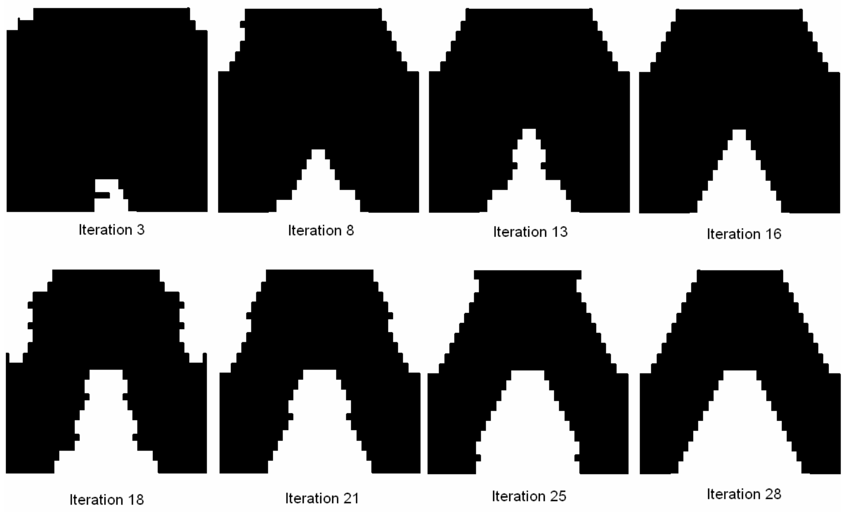


Figure 5. Evolution history for orthotropic material – Case B.

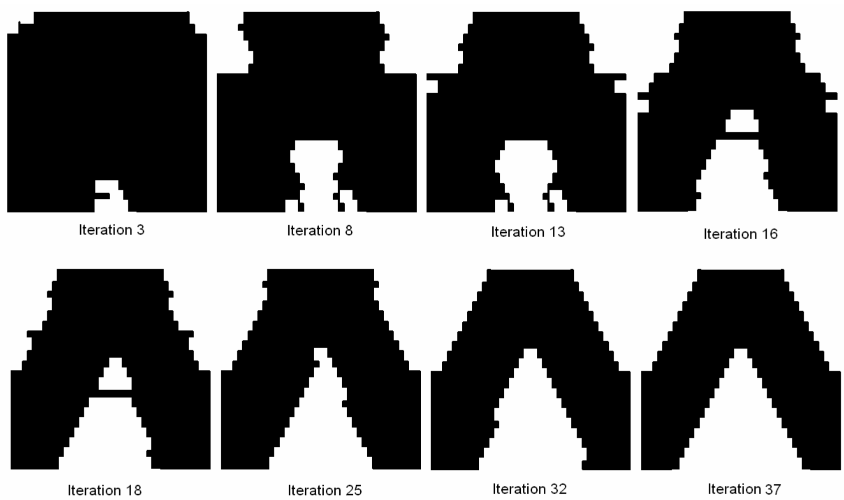


Figure 6. Evolution history for orthotropic material – Case C.

Figure 8 presents the evolution of the material removal for all cases. It was found that highly orthotropic cases result higher values of the topological sensitivity, in comparison to its isotropic solution. Consequently, a larger material removal rate is expected for orthotropic problems, in general, but this is a very problem dependent assertion.

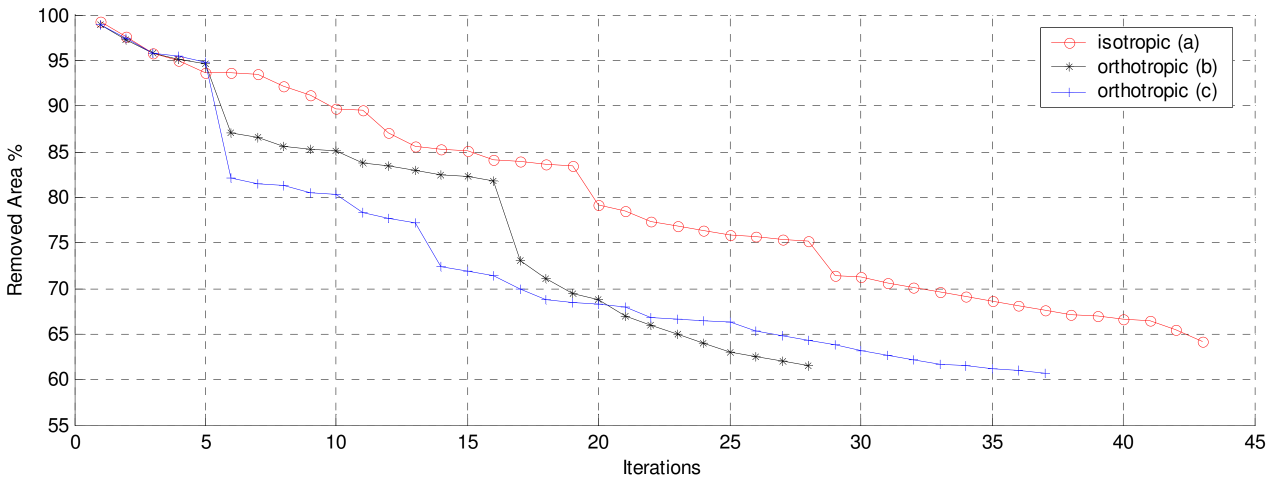


Figure 7. Material removal history for example 2.

5.3 Example 3 – Cross heat conductor

This example refers to a square domain subjected to low and high temperature boundary conditions on the middle of opposite sides. The problem is depicted in Figure 8, where T_H is the high temperature (373 K) and T_L is the low temperature (273 K). The remaining boundaries are insulated. All possible cases will be studied: isotropic, orthotropic and anisotropic materials. All cases are to be optimized until $A_f \approx 0.4\, A_0$ is achieved.

Initially an isotropic case was analyzed with $k_{11} = k_{22} = 1$. Symmetry was not used to provide a direct comparison to the subsequent anisotropic cases (which cannot use symmetry). Figure 8 shows the evolution of material removal for $r = 0.02 l_{ref}$. It is important to note that the algorithm delivered fairly symmetric solutions throughout the process. The condition $A_f \approx 0.4\, A_0$ was achieved after 34 iterations.

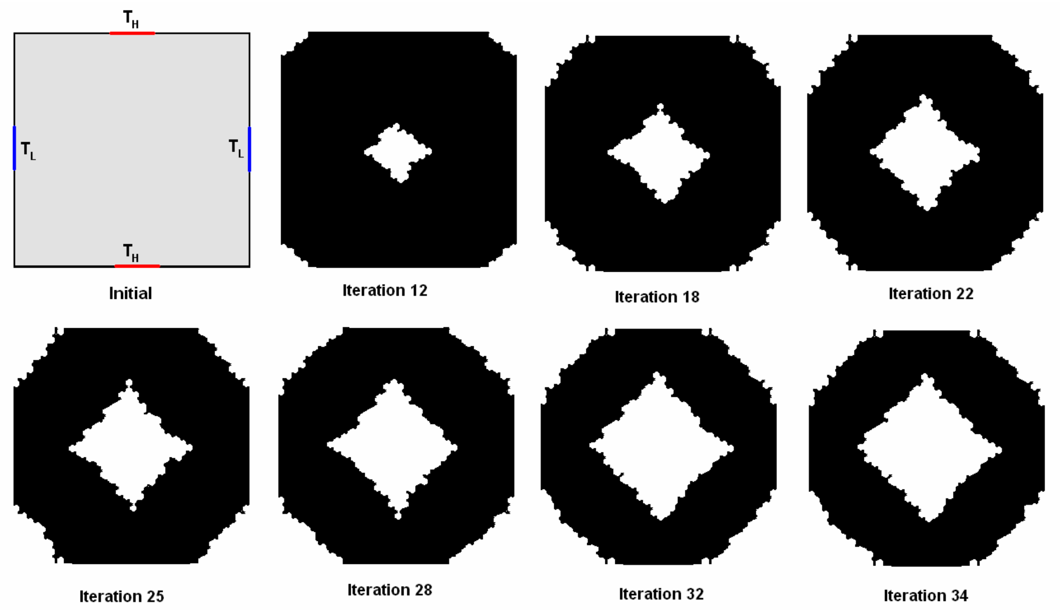


Figure 8. Evolution history for example 3 – isotropic case.

The second case represents a highly orthotropic material, with the conductivities set to $k_{xx} = 5$ and $k_{yy} = 1$. As expected, material is selectively removed so that the heat flux along the x direction is majored. The stop criteria $A_f \approx 0.4\, A_0$ was achieved after 30 iterations.

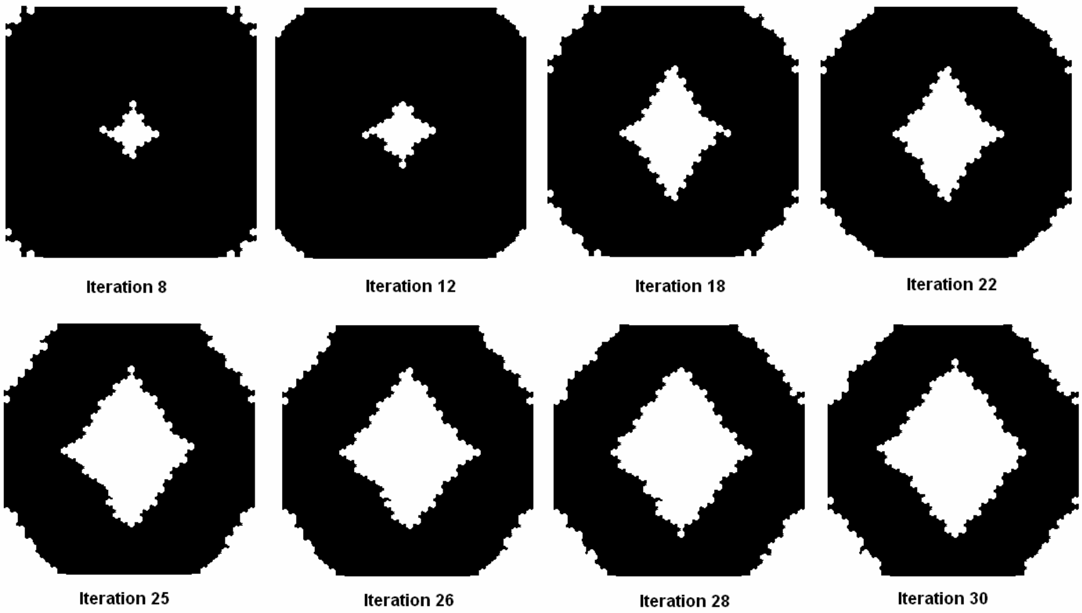


Figure 9. Evolution history for example 3 – orthotropic case.

The third case considers an anisotropic material with k_{xx} = 1, k_{yy} = 1 and k_{xy} = 0.5. The evolution history is presented in Fig.11, showing that the initial symmetry is lost after the first iterations, as expected. Contrary to the previous cases, the internal cavity resulted in a rhombic shape, since the Cartesian axes are not parallel to the principal axes of the constitutive matrix.

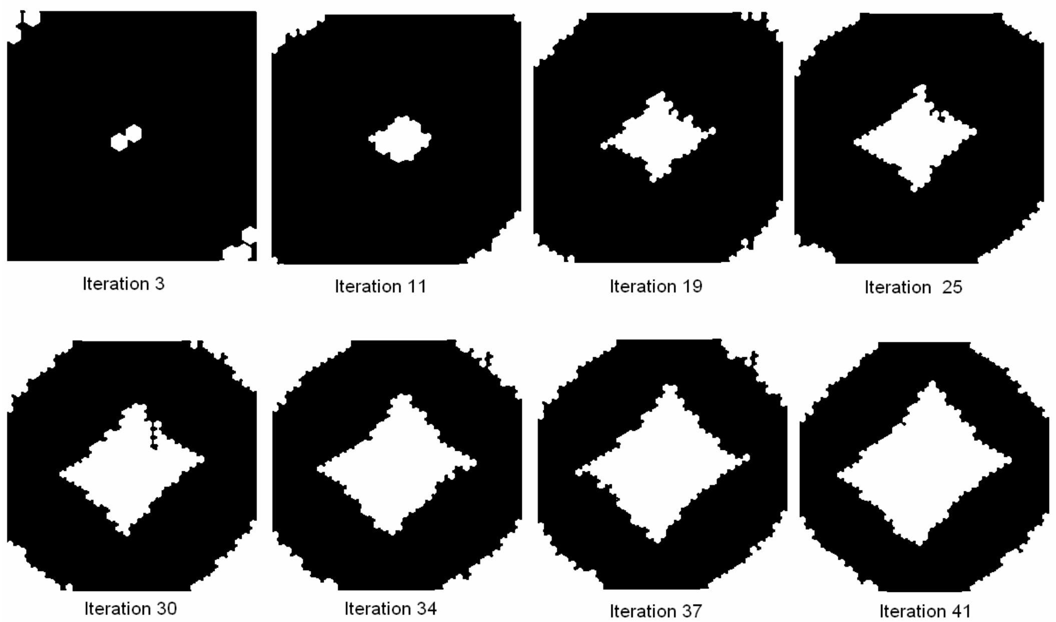


Figure 10. Evolution history for example 3 – anisotropic case.

Figure 11 shows the percentage of material removed versus the number of iterations for each case studied in example 3. All cases were stopped when about 40% of material was removed. These cases were analyzed without the aid of symmetry, for comparison purposes. Obviously, anisotropic cases cannot use symmetry in general, but in many practical situations it is possible (or even desirable) to align the axes of the component with the principal directions of the constitutive matrix. In such cases, more smooth designs can be obtained.

In order to provide a further benchmark, example 3 was re-analyzed for the isotropic and orthotropic cases using only one quadrant of the original geometry. Figure 13 show the final topologies obtained for both cases. The material was removed initially with r = 0.04 l_{ref} and r = 0.02 l_{ref}. for the remaining iterations. This simple expenditure helps to generate smoother boundaries in the final design.

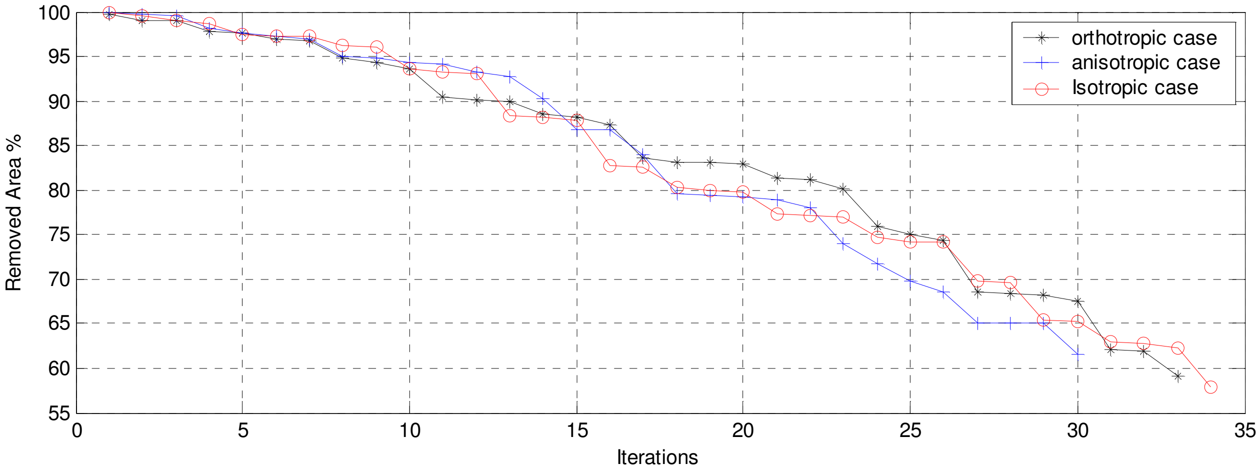
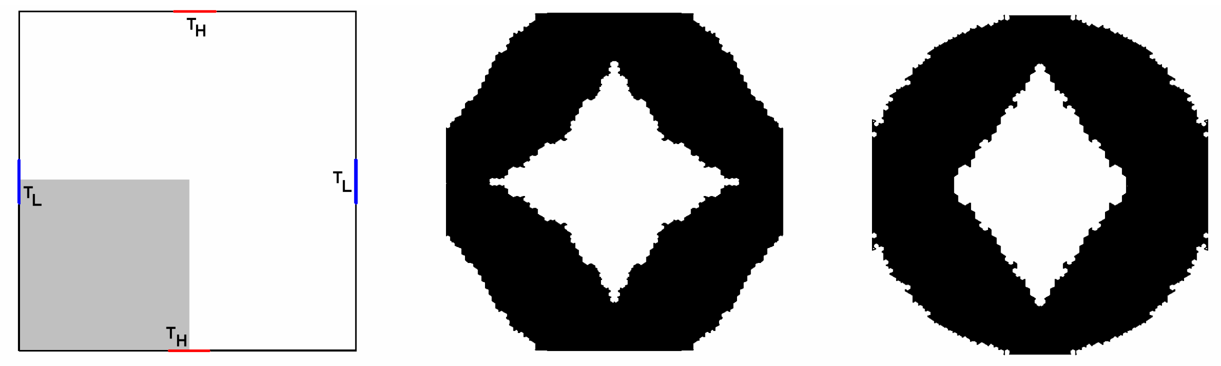


Figure 11. Material removal history for example 3.



(a) (b)

Figure 12 – Final topologies for: (a) isotropic and (b) orthotropic examples.

6. Conclusions

The objective of this paper is to extend a previous 2D heat transfer BEM topology optimization implementation (Marczak, 2005) to anisotropic constitutive behavior. A linear coordinate transformation method was implemented in order to allow the use of DT, since this formulation was deduced only for isotropic materials. The cost function (potential energy density) is not explicitly given, and extensions of the formulation for other types of cost function will demand elaborate analytical derivations. Some BEM and DT characteristics were preserved as: no domain mesh, absence of intermediary material densities, unnecessary application of filters in the pos-processing, and low computational cost. The methodology developed in this paper is an elegant way to extend the DT approach to non-isotropic materials, avoiding new analytical derivations. Some cases of linear heat transfer were solved showing the feasibility of the proposed procedure and good agreement with other solutions.

7. Acknowledgements

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