# ADAPTING THE SIMP MODEL FOR TOPOLOGY OPTIMIZATION OF BIOMECHANICAL STRUCTURES

**Jonatan Rivilla Álamo, jonrivala@gmail.com**
**Francisco Ilson da Silva Junior, ilson@ufc.br**
Department of Mechanical Engineering, Federal University of Ceará (UFC) Campus do Pici - Bloco 714 - CEP 60455-760 Fortaleza, Ce, Brazil

***Abstract.*** *This paper presents a solid isotropic material penalization model (SIMP) based topology optimization research and its subsequent adaptation, which allows to obtain one similar method for ortotropic materials. Both methods have been used in the development of a regeneration model that finally has been applied to the research of the evolution of the bone, after an operation of artificial hip (prosthesis). This way, the present research shows different areas of knowledge, facts that have been introduced starting with a short and general historical introduction. This areas have become more focused in the idea of obtaining key concepts, in order to define the topic. The research themes are Optimization, the Finite Element Method and Biomechanics. In this work, a numerical problem is solved. The case study is a post-operative femur after a femoral head is replaced by a prosthesis metallic. A preliminary contact model is developed for load application on the femoral structure. The goal of this study is to determine the bone tissue regeneration around the prosthesis due to adaptation of the loads. Thus, a more efficient design of the prosthesis can be obtained. By analysis of the material density results, some aspects of bone regeneration can be clarify. It can be concluded that the topology optimization proposed can be assumed an important tool to support medical applications of bone assessment.*

***Keywords:*** *bone regeneration, orthotropic materials, finite element modeling*

## 1. INTRODUCTION

The bone regeneration topic has been an important research topic for last years by researchers in biomechanical themes. The goal of this paper is to propose a systematic methodology to model the regeneration of bones in processing of metallic implants. In this context, mathematical optimization methods were used in order to predict the process of bone calcification through biomechanical models. The optimization process can be understood as the search of good solutions for state variables that describing the behavior of any nature system. This way, the optimal solution is one of the best according to some specific criterion. In general, the feasible solution domain are composed by a series of restrictions or requirements. Topology Optimization is frequently used to design mechanical structures systems in a large range of engineering applications. Pioneering works in finite element based topology optimization were developed by Bendsoe and Kikuchi (1988), Bendsoe (1989) and Susuki and Kikuchi (1991). They used the homogenization method to find the best distribution of material and holes in several structures. In structural optimization and design, some topology optimization techniques have been intensively used to solve compliance minimization problems (Xie and Steven, 1997; Sigmund and Jensen, 2003; Hsu and Hsu, 2005). The authors used a methodology based on interpolation scheme. Among others works, Evolutionary Algorithms (EA) have demonstrated efficiency and accuracy to find optimal solutions for a large range of optimization problems (Xie and Steven, 1997; Farmani *et al.*, 2005). In this work, the analysis of the bone regeneration process is done by different approaches. First of all, it is performed the topology optimization process. This way, it is established an objective function that represents the biological loading on bone tissue. In order to predict the adaptation of bone subjected to mechanical loads, it is determined one mathematical relationship among stimulus and response of bone material. The other approach is mechanistic. In other words, the bone adaptation from cell biology is adapted by natural models, in focus on the tissue system (Garzon *et al.*, 2005). The topology optimization, more specifically can be applied intuitively in analysis of bone regeneration, taking into account some considerations to fit the general model to this specific application.

The outline of the rest of the paper is as follows. In Section 2, the optimization concepts are stated. In the next section, the elastic bone-structure model is described. Moreover, the basic assumptions are presented and the isotropic and orthotropic elastic behaviors are presented by constitutive equations description. In this context, the numerical approaches applied to find the material distribution in a regeneration bone process is presented. This way, some formulations to solve optimization problem are discussed. In Section 4, the numerical results are presented and the performance of the method is illustrated. The conclusions are outlined in Section 5.

## 2. OPTIMIZATION PROBLEM STATEMENT

In general, the systems has different responses to the causal relations. Therefore, it is necessary to analyze them to determine which is most desirable. Any mathematical model that involves the search for best responses of systems, among all possible, it is classified as an optimization model (Otero *et al.*, 2006). This way, in Eq. (1), the general formulation of the optimization problem is done as follows (Bazaraa *et al.*, 2006):

$$\begin{aligned} &\text{Min } f(x) \\ &\text{such as: } x \in S \end{aligned} \quad (1)$$

where $x$ represents the design variables, $f(x)$ is the objective function and the set $S$ is describe by equalities and inequalities, $h_i(x)$ and $g_j(x)$, respectively. In Equation (2), the mathematical statement for the feasible region $S$ is presented.

$$\begin{aligned} &S \equiv \{x \in \Omega / h_i(x) = 0;\ g_j(x) \leq 0\} \\ &\text{such as} \\ &i \in I = \{1, 2, ...m\} \\ &j \in J = \{1, 2, ..., k\} \end{aligned} \quad (2)$$

where the set $\Omega$ correspond to the state variable values in a finite dimension.

The topology optimization of the bone-structure system is performed using an continuum model for the material that combines a finite element method with an optimality criteria optimization technique. The objective of this optimization is to find the material distribution history of bone-structure domain $\Omega$ for a particular boundary conditions setting. The finite element formulation implemented is based on the differential equations of plane elasticity based on the displacements values for isotropic and orthotropic material behavior (Cook *et al.*, 2001). In the next section, the SIMP ("Solid Isotropic Material with Penalization") and SOMP ("Solid Orthotropic Material with Penalization") methods are developed in the context of the bone regeneration problem.

## 3. BONE REGENERATION MODEL

In this section, it is presented the model of bone regeneration by topology optimization. However, our objective is not build a model that faithfully simulates the reality, but provide an initial draft about a possible research line.

The human body has four mechanisms that control the dynamic changes of bone: growth, modeling, remodeling and bone repair (Hernandes *et al.*, 1995). In this work, the focus is the bone remodeling. In this process, certain areas of bone are destroyed and replaced by new bone tissue. In the bone remodeling process, structural changes leading to an increased sensitivity to mechanical stimuli because the bone-structure system can accumulate fatigue damage or micro fractures. In view of structural modification process controlled by the remodeling to adapt to possible changes in mechanical stimuli, the use of the SIMP model for regeneration and placement of bone is justified. On the other hand, it is created a laminated tissue oriented along the lines of force acting on the area being repaired. This leads to the use of orthotropic models like as the SOMP model proposed.

The design variable is defined as the relative density between the solid material and empty regions. This variable must be evaluated in the domain. In this context, the design variables are defined as elementary densities and "gray" solutions are allowed. In other words, for structural optimization case, it is necessary to obtain solutions with defined solid shapes. However, for the bone regeneration case, the optimization is free to distribute the material in the domain with the best configuration as possible, including densities values among 0 and 1.

The SIMP formulation is considered easy implementation in the context of a finite element program. There are explicit procedures for evaluating the relative densities. This way, the resolution of the minimizing problem is facilitated (Bendsoe, 2005; Muiños, 2001). However, the classical SIMP method can present numerical instabilities. For this reason, the convergence of the method is prevented and it leads to distributions known as "checkerboard".

For the bone regeneration model, another design variable is introduced to the optimization model. Because the existence of a preferred direction of bone growth, the variable $\theta$ is introduced. It is supposed that the mechanism of regeneration is free to replace the directions of the blades in any direction and quantity, for both macroscopic and microscopic scales. In accordance with this theory, the physical properties in the direction $\theta$ are different values when compared with the properties of others directions. The SOMP formulation can be understood as a SIMP model modified by using orthotropic material models.

### 3.1 Finite element description

In this paper, is is supposed small displacement values and the loads acting on the material in the linear elastic field. The elastic domain $\Omega$ is discretized by quadrilateral elements with linear shape functions (Cook *et al.*, 2001; Reddy, 1984). Using Galerkin's method in the plane elasticity equations and taking $\delta\mathbf{U}$ as the admissible virtual variation of the structural displacement vector **U**, we can define the strain tensor operator applied to structural displacement variable, as follows:

$$\varepsilon(\mathbf{U}) = \mathbf{B}(x,y)\mathbf{U} \tag{3}$$

where $\mathbf{B}(x,y)$ is the differential operator to plane elasticity problem.

The tensor of stress $\sigma$ is related with the tensor of strain by linear constitutive equation, in the following form:

$$\sigma(\mathbf{U}) = \mathbf{C}\,\varepsilon(\mathbf{U}) \tag{4}$$

where **C** is the constitutive matrix.

In the equilibrium, the internal forces can be grouped in a integral formulation. For a finite element domain $\Omega_e$, the virtual internal work $W_i$ can be evaluated by Eq. (5).

$$W_i = \int_{\Omega_e} \varepsilon^t(\delta\mathbf{U})\sigma(\mathbf{U})d\Omega \tag{5}$$

Finally, substituting the Eq. (3) and (4) into (5), using a finite element approximation for **U** and $\delta\mathbf{U}$ and isolating the elementary stiffness matrix, we obtain:

$$K_e = \int_{\Omega_e} \mathbf{B}^t(x,y)\,\mathbf{C}\,\mathbf{B}(x,y)\,d\Omega \tag{6}$$

The Equation (6) is used to calculate the elementary contribution. Therefore, the global assemblage is performed and a linear system problem is produced. In order to obtain the global displacement **U**, the linear equation system must be solved for instance using numerical methods. In the next section, it is presented the particularities for the isotropic and orthotropic formulations. The relevant constitutive relations are presented in Section 3.2

### 3.2 Constitutive equations for elastic materials

In this work, it is assumed plane stress formulation. For isotropic material behavior, the constitutive matrix is done as:

$$C_1 = \frac{E}{1-\nu^2}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{bmatrix} \tag{7}$$

where the material properties are the Young Modulus $E$ and the Poisson's ratio $\nu$.

The orthotropic materials are composed by blades arranged in orthogonal directions as description in Fig. 1. A few number of material constants are used to represent the constitutive matrix for orthotropic materials (Haftka and Gürdal, 1991).

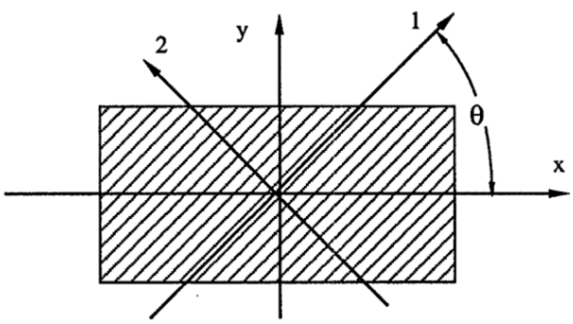



Figure 1. The blade direction in the orthotropic material

In this context, we introduce $\theta$ as the direction of blades to respect the global axis $x$. The constitute matrix for orthotropic materials in a plane state is presented as follows:

$$C_2 = \begin{bmatrix} \bar{Q}_{11} & \bar{Q}_{12} & \bar{Q}_{16} \\ \bar{Q}_{12} & \bar{Q}_{22} & \bar{Q}_{26} \\ \bar{Q}_{16} & \bar{Q}_{26} & \bar{Q}_{66} \end{bmatrix} \tag{8}$$

In Equation (9) through (14), it is presented the terms of the constitutive matrix $C_2$.

$$\bar{Q}_{11} = Q_{11}\cos^4\theta + 2(Q_{12} + 2Q_{66})\sin^2\theta\cos^2\theta + Q_{22}\sin^4\theta \tag{9}$$
$$\bar{Q}_{12} = (Q_{11} + Q_{22} - 4Q_{66})\sin^2\theta\cos^2\theta + Q_{12}(\sin^4\theta + \cos^4\theta) \tag{10}$$
$$\bar{Q}_{22} = Q_{11}\sin^4\theta + 2(Q_{12} + 2Q_{66})\sin^2\theta\cos^2\theta + Q_{22}\cos^4\theta \tag{11}$$
$$\bar{Q}_{16} = (Q_{11} - Q_{12} - 2Q_{66})\sin\theta\cos^3\theta + (Q_{12} - Q_{22} + 2Q_{66})\sin^3\theta\cos\theta \tag{12}$$
$$\bar{Q}_{26} = (Q_{11} - Q_{22} - 2Q_{66})\sin^3\theta\cos\theta + (Q_{12} - Q_{22} + 2Q_{66})\sin\theta\cos^3\theta \tag{13}$$
$$\bar{Q}_{66} = (Q_{11} + Q_{22} - 2Q_{12} - 2Q_{66})\sin^2\theta\cos^2\theta + Q_{66}(\sin^4\theta + \cos^4\theta) \tag{14}$$

where the orthotropic terms $Q$ are calculated using the material constants measures in orthogonal directions 1-2. The relations are presented as follows:

$$Q_{11} = \frac{E_1}{1 - \nu_{12}\nu_{21}} \tag{15}$$
$$Q_{22} = \frac{E_2}{1 - \nu_{12}\nu_{21}} \tag{16}$$
$$Q_{12} = \frac{\nu_{12}E_2}{1 - \nu_{12}\nu_{21}} = \frac{\nu_{21}E_1}{1 - \nu_{12}\nu_{21}} \tag{17}$$
$$Q_{66} = G_{12} \tag{18}$$

In the next section, it is presented a description of the SIMP and SOMP optimization models based on development done by Sigmund (2001).

### 3.3 The Compliance Minimization Problem

The structural optimization can be applied under different approaches: minimization of stress, strain, weight, etc. The minimization of the internal energy is proposed by Bendsoe and Kikuchi (1988) as equivalent to stiffness maximization. In this work, the objective function is the compliance of the structural system $c(x)$. This optimization problem correspond to determine the best material distribution that presents the bigger stiffness/weight ratio. Therefore, the objective function in a finite element formulation can be written as:

$$\begin{array}{l} \text{Min}\, c(x) = \mathbf{U}^t\mathbf{K}\mathbf{U} = \sum\limits_{e=1}^{N} x_e^p u_e^t k_e u_e \\ \text{such as:} \\ V(x)/V_0 = f \\ \mathbf{KU} = \mathbf{F} \\ 0 < x < 1 \end{array} \tag{19}$$

where **U** represents the nodal vector displacement, **K** is the global stiffness matrix, $N$ is the number of elements in the mesh, $x_e$ is the density of element $e$, $p$ is the penalty value, $u_e$ is the nodal vector displacement evaluated in the nodes of the element $e$, $k_e$ is the element stiffness matrix, $f$ is the volumetric fraction of material, $V_0$ is the initial volume of material.

The optimization process is based on the gradient of the objective function value with respect to elementary densities (optimality criteria method). The evaluation of the design variables $x$ is done by the algorithm as follows:

$$x_e^{new} = \begin{cases} \max(x_{\min}, x_e - m) \\ \text{if} x_e B_e^\eta \leq \max(x_{\min}, x_e - m), \\ x_e B_e^\eta \\ \text{if } \max(x_{\min}, x_e - m) < x_e B_e^\eta < \min(1, x_e + m), \\ \min(1, x_e + m) \\ \text{if } \min(1, x_e + m) \leq x_e B_e^\eta \end{cases} \tag{20}$$

where $m$ is a positive limit number to $x_e$, $\eta$ works as damping factor. The function $B_e$ indicates the direction of the minimum solution and it defined as:

$$B_e = \frac{-\partial c/\partial x_e}{\lambda\,\partial V/\partial x_e} \tag{21}$$

where $\lambda$ is the Lagrange multiplier. In this context, the gradient function of the compliance $c(x)$ is done by:

$$\frac{\partial c}{\partial x_e} = p\,x_e^{p-1} u_e^t k_e u_e \tag{22}$$

In order to overcome the checkerboard distribution problem, Sigmund (1997) introduces a new gradient function calculated by using filtering properties, as described in Eq. (23).

$$\widehat{\frac{\partial c}{\partial x_e}} = \frac{1}{x_e \sum\limits_{f=1}^{N} \widehat{H}_f} \sum_{f=1}^{N} \widehat{H}_f x_f \frac{\partial c}{\partial x_f} \tag{23}$$

where $\widehat{H}_f$ is a convolution operator done by:

$$\begin{array}{l} \widehat{H}_f = r_{\min} - dist(e,f), \\ \{f \in N/dist(e,f) \leq r_{\min}\}\,, e = \{1,...,N\} \end{array} \tag{24}$$

For the SOMP method, several meshes must be build to represent the behavior of each orthotropic blade. In Figure (2), it is presented the several blade directions of the orthotropic material for optimization analysis using the SOMP method.

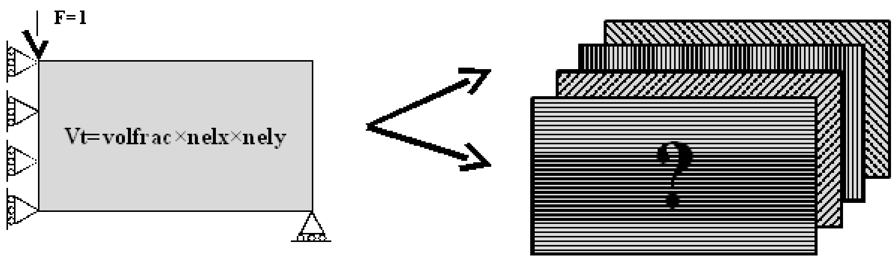



Figure 2. Several planes configurations for the orthotropic material optimization

In order to determine the global stiffness matrix for the SOMP optimization method, sub-elements matrices corresponding to several direction blades are calculated. Therefore, the elementary stiffness matrix is update as:

$$K_e = \sum_{i=1}^{n_b} K_{e,\theta_i} \tag{25}$$

where $K_{e,\theta_i}$ represents the sub-element matrix in the direction $\theta_i$ and $n_b$ is the number of available blades to model.

In this context, the optimization formulation presented can be considered appropriate since the cell system in regeneration acts constantly. This construction process has been demonstrated in several experimental studies (Cojín, 2001). In the next section, the optimization methods are performed by numerical tests. A geometrical model of a typical femoral bone is obtained and submitted to regeneration process analysis.

## 4. NUMERICAL RESULTS

In this section, the numerical results of plane elastic domains for two material behaviors are presented. The SIMP and SOMP methods were applied in order to determine the probably configuration of a femoral bone in regeneration after implant procedure. In Figure (3), a typical radiography of femoral bone with metallic implant and boundary conditions of domain are presented. By geometrical analysis, the dimensions of the bone domain were estimated. The external forces were introduced based on typical values of body solicitations studies, but there is not accuracy about the contact model. Therefore, the bigger loading situation on the bone was used.

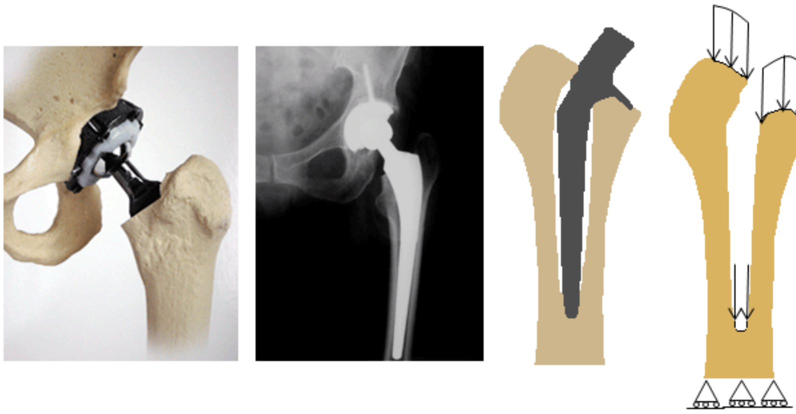
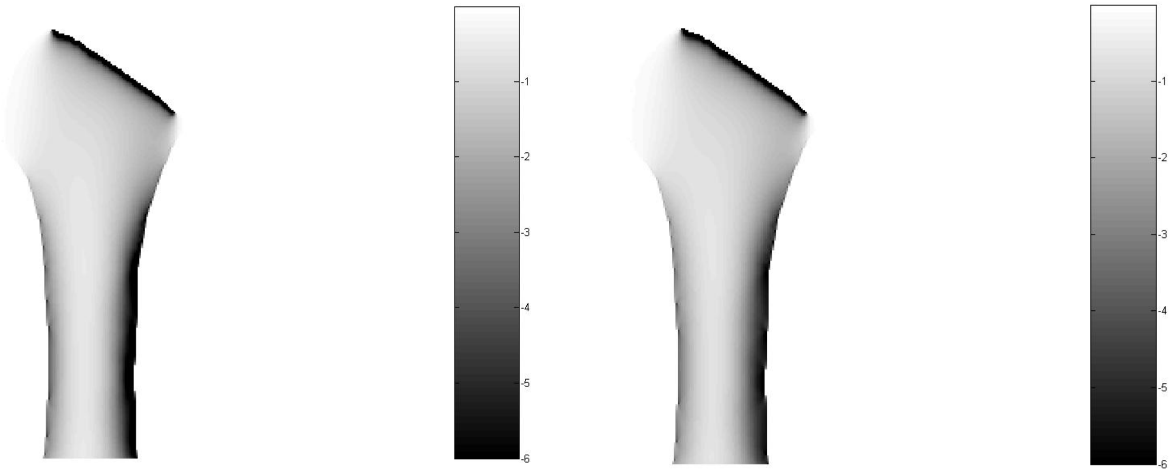


Figure 3. Femoral bone domain and its boundary conditions

The first test consists in evaluate the bone regeneration process in a domain without the presence of implants. For SIMP and SOMP model, it was removed 50% of initial volume material, the following results are obtained, as described in Fig. (4).

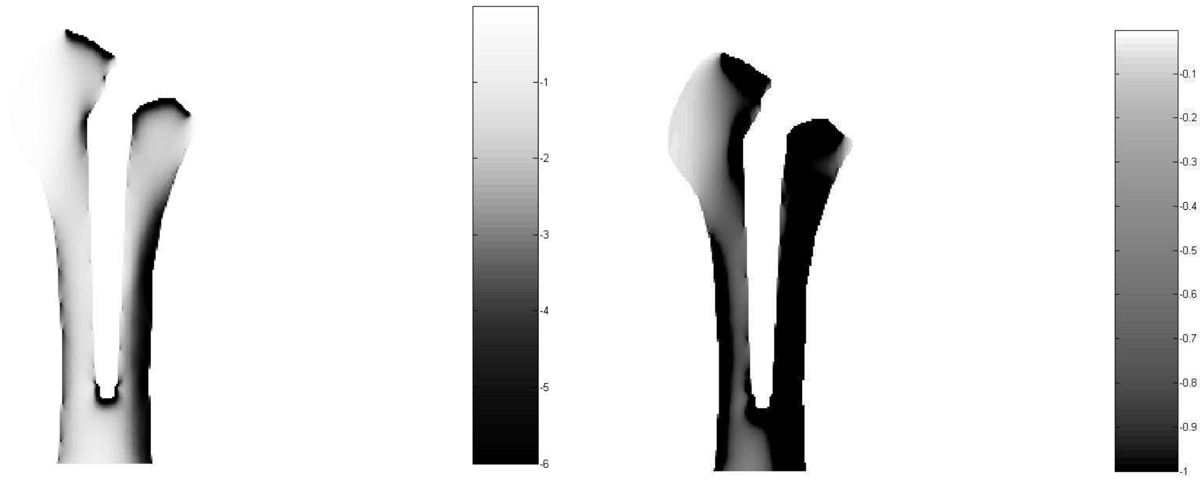



(a) density distribution - SIMP method
volume reduction ratio $f = 0.5$
compliance value $c = 186.3$

(b) density distribution - SOMP method
volume reduction ratio $f = 0.5$
compliance value $c = 225.5$

Figure 4. Optimization results without implant presence.

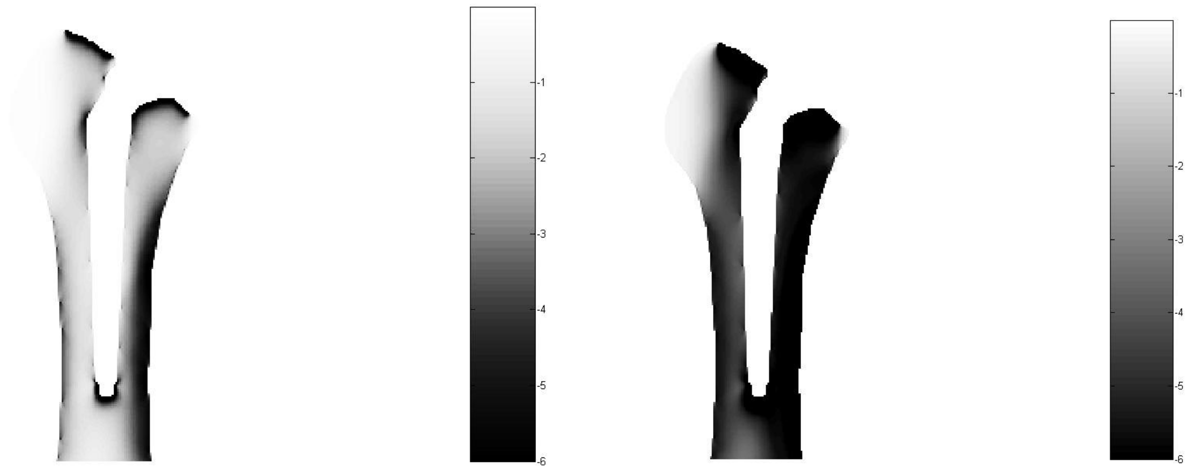
For the second test, the implant presence case was analyzed. Firstly, the bone material was considered isotropic. The optimization results are presented in Fig. (5). For the last test, the bone material was considered orthotropic and the SOMP method was used. For this case, the optimization results are presented in Fig. (6).




(a) density distribution - SIMP method
volume reduction ratio $f = 0.5$
compliance value $c = 211.9$

(b) density distribution - SIMP method
volume reduction ratio $f = 0.8$
compliance value $c = 174.8$

Figure 5. Optimization results with implant presence - Isotropic Material Behavior.




(a) density distribution - SOMP method
volume reduction ratio $f = 0.5$
compliance value $c = 256.1$

(b) density distribution - SOMP method
volume reduction ratio $f = 0.8$
compliance value $c = 221.5$

Figure 6. Optimization results with implant presence - Orthotropic Material Behavior.

It can be noted similar results for the SIMP and SOMP models. Global results were found for both models regarding density distribution on the domain. However, the compliance values of optimal solutions are different. For the ortotropic material case, it was used 10% of relative difference among the properties in the orthogonal directions. For the implant presence case, it was obtained a relative diference of 26,7% on the SIMP and SOMP compliance results. The penalty value used was $p = 3$, and it is responsible to obtain the density distributions presented.

Due to some regions have presented density values lower to corresponding regions in the analysis without implant presence, the need of new prosthesis design can be relevant. This way, the load on the bone should be differently transmitted. Therefore, a new study can be performed: the topology optimization of the metallic implant.

## 5. CONCLUSIONS

In this work, a bone regeneration model as optimization process have been proposed. A geometrical configuration obtained from computerized images was used to build the domain discretized by plane finite elements. In this context, a femoral bone with metallic implants presence has been analyzed by several numerical tests. It was created a first methodology to detect the recuperation of bone tissue systems. The main objective is select and evaluate the application of prosthesis in clinical cases. Therefore, the topology optimization can be a useful tool for aid the Medical Research on the bone regeneration evaluation. This work has a qualitative aspect and the results make up some future researches themes. Further works will include multi-physics modeling, three-dimensional analysis and studies about the governing parameters of the bone regeneration mechanisms.

## 6. ACKNOWLEDGEMENTS

The authors would like to thank CNPq (Conselho Nacional de Pesquisa - Brasil) for financial support for this work .

## 7. REFERENCES

Bazaraa, M.S., Sherali, H.D. and Shetty, C.M., 2006. *Nonlinear Programming: Theory and Algorithms*. John Wiley and Sons, New Jersey.

Bendsoe, M.P., 2005. *Optimization of structural topology, shape, and material*. Springer-Verlag, Heidelberg.

Bendsoe, M.P., 1989. “Optimal shape design as a material distribuition problem”. *Structural Optimzation*, Vol. 1, pp. 193–202.

Bendsoe, M.P. and Kikuchi, N., 1988. “Generating optimal topologies in structural design using a homogenization method”. *Computer Methods in Applied Mechanics and Engineering*, Vol. 71, pp. 197–224.

Cojín, S., 2001. *Bone mechanics handbook*. CRC Press Boca Raton, USA.

Cook, R.D., Malkus, D.S., Plesha, M.E. and Witt, R.J., 2001. *Concepts and Applications of Finite Elements Analysis - Fourth Edition*. John Wiley and Sons, Inc., University of Wisconsin - Madison.

Farmani, R., Savic, D.A. and Walters, G.A., 2005. “Evolutionary multi-objective optimization in water distribution network design”. *Engineering Optimization*, Vol. 37 (2), pp. 167–183.

Garzon, D.A., Roa, A.M. and Duque, C.A., 2005. “Analisis del regeneramiento óseo bajo el esquema de la optimización topológica”. *Ingeniería e Investigación - Universidad Nacional de Colombia, Colombia*, Vol. 25 (1), pp. 167–183.

Haftka, T. and Gürdal, Z., 1991. *Elements of Structural Optimization*. Kluwer Academic Publishers, University of Virginia.

Hernandes, J., Serrano, S., Marinoso, M., Aubia, J., Lloreta, J. and J. Marrugat, A.D., 1995. “Bone growth and modeling changes induced by periosteal stripping in the rat”. *Clinical Orthopedic*, Vol. 320, pp. 211–219.

Hsu, M.H. and Hsu, Y.L., 2005. “Generalization of two- and three-dimensional structural topology optimization”. *Engineering Optimization*, Vol. 37 (1), pp. 83–102.

Muiños, I., 2001. *Optimización Topológica de Estructuras: Una Formulación de Elementos Finitos para la Minimización del Peso con Restricciones en Tensión*. Proyecto Técnico, ETSICCP, Universidad de A. Coruña.

Otero, J.M., Kaves, A. and Marrero, A., 2006. *Modelos de optimización continuos*. Editorial Félix Varela, Havana, Cuba.

Reddy, J.N., 1984. *An Introduction to the Finite Element Method*. MacGraw-Hill, New York.

Sigmund, O., 2001. “A 99 line topology optimization code written in matlab”. *Structure Multidisciplinar Optimization*, Vol. 21, pp. 120–127.

Sigmund, O. and Jensen, J.S., 2003. “Systematic design of phononic band-gap materials and structures by topology optimization”. *Philosofy Transactions of Royal Society*, Vol. 361, pp. 1001–1019.

Sigmund, O., 1997. “On the design of compliant mechanisms using topology optimization”. *Mechanics of Structures and Machines*, Vol. 25, No. 4, pp. 495–526.

Susuki, K. and Kikuchi, N., 1991. “A homogenization method for shape and topology optimization”. *Computer Methods in Applied Mechanics and Engineering*, Vol. 93, pp. 291–318.

Xie, Y. and Steven, G., 1997. *Evolutionary Structural Optimization*. Springer Verlag.