

4th International Conference on Tissue Engineering, ICTE2015

## Combined Elastic and Shear Stress Solicitations for Topological Optimisation of Micro-CT Based Scaffolds

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### Abstract

Advanced additive manufacturing technologies, namely Biomanufacturing, are being used to fabricate scaffolds with controlled architecture for tissue engineering applications. These technologies combined with computer-aided design (CAD) enable to produce three-dimensional structures layer-by-layer in a multitude of biomaterials. Actual prediction of the effective mechanical properties of scaffolds produced by Biomanufacturing, is very important for tissue engineering applications. A novel computer based technique for scaffold design is topological optimisation. Topological optimisation is a form of “shape” optimisation, usually referred to as “layout” optimisation. The goal of topological optimisation is to find the best use of material for a body that is subjected to either a single load or a multiple load distribution. In this research work, a topological optimization strategy is presented to find out the best material use for a construct subject to either a single load or a multiple load distribution, maximising its mechanical behaviour under tensile and shear stress solicitations. The proposed topological optimization scheme enables the design of ideal topological architectures based on existing biologic Micro-CT data for the design of biomimetic scaffolds.

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Peer-review under responsibility of IDMEC-IST

*Keywords:* Computational technologies; Topological optimization; Tissue engineering; Scaffolds; Micro-CT data.

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## 1. Introduction

In tissue engineering, the formation of tissues with desirable properties strongly relies on the mechanical properties of the scaffolds at a macroscopic and microscopic level. Macroscopically, the scaffold must bear loads to provide stability to tissues while it is being formed fulfilling its volume maintenance function. At the microscopic level, both cell growth and differentiation and ultimate tissue formation are dependent on the mechanical input to cells. Thus, the scaffold must be able to withstand specific loads and transmit them in an appropriate way to the growing and surrounding cells and tissues [1-3].

The design of optimised scaffolds for tissue engineering is a key topic of research, as the complex macro- and micro- architectures required for a scaffold depends on the mechanical properties, physical and molecular queues of the surrounding tissue at the defect site. One way to achieve such hierarchical designs is to create a library of unit cells (the scaffold is assumed to be a “Lego” structure), which can be assembled through a specific computational tool [4-6].

In this research work, a topological optimization strategy is presented to find out the best material use for a construct subject to either a single load or a multiple load distribution, maximising its mechanical behaviour under tensile and shear stress solicitations. The proposed topological optimization scheme enables the design of ideal topological architectures based on existing biologic Micro-CT data for the design of biomimetic scaffolds.

## 2. Topological Optimisation

The classical problem in engineering design consists in finding the optimum geometric configuration of a structure that maximizes a given cost objective function with boundary conditions and constraints. Structural optimisation can be classified as follows [7,8]:

- Size optimisation;
- Shape optimisation;
- and Topology optimisation.

In size optimisation, only the cross section of a structure is optimised. A typical size feature of a given structure, such as the thickness of a beam, is either increased or decreased in order to improve its performance. In shape optimisation, the shape of the structure is obtained by changing the shape of the used components with other components of different shape, in order to improve a desired variable within a system. In topology optimisation, the shape and connectivity of the domain are both design variables.

Topology optimisation provides the first design concept of the structure’s materials distribution. Its goal is to minimise the structure compliance while satisfying the constraints of volume removal. As the structure compliance is twice the strain energy, the objective function of minimising structure compliance is equivalent to minimising strain energy [9,10].

In spite of several attempts to define optimised scaffolds [11-16], there is no work correlating both porosity and mechanical properties with topological information. Scaffolds must be highly porous structures but also effective from a mechanical point of view. This is a complex issue, fundamental for tissue engineering applications and not yet fully addressed. This paper proposes an optimised strategy to obtain scaffolds with an appropriate topology maximizing both porosity and mechanical behaviour. The methodology proposed in this paper is of simple implementation and does not require high computational calculation time.

### 2.1. Topological Optimisation

Topological optimisation, aiming to find the best use of material according to a “maximum-stiffness” design, requires neither parameters nor the explicit definition of optimisation variables. The objective function is predefined, as are the state variables (constrained dependent variables), and the design variables (independent variables to be optimised). The topological optimisation problem requires the problem definition (material properties, model and loads), the objective function (the function to be minimized or maximized), and the state variables corresponding to the percentage of material to be removed [8-10,17-18].

From a mechanical point of view, the goal of topological optimisation is to minimise the total compliance, which is proportional to the strain energy. Figure 1 illustrates the general topology optimisation scheme considered in this work.

The design variables are internal, pseudo-densities that are assigned to each finite element in the topological problem. The pseudo-density for each element varies from 0 to 1, where  $\eta_i \approx 0$  represents material to be removed, and  $\eta_i \approx 1$  represents material that should be.

For a given domain  $\Omega \subseteq \mathfrak{R}^2(\mathfrak{R}^3)$ , regions  $\Omega(\Gamma_i)$  and fixed boundaries, the optimisation goal is to find the optimal elasticity tensor  $E_{ijkl}(x)$ , which takes the form [20-22]:

$$E_{ijkl}(x) = \eta(x) \bar{E}_{ijkl} \quad (1)$$

where  $\bar{E}_{ijkl}$  is the constant rigidity tensor for the considered material and  $\eta(x)$  is an indicator function for a region  $\Omega^* \subseteq \Omega$  that is occupied by material:

$$\eta(x) = \begin{cases} 1 & , \text{ if } x \in \Omega^* \\ 0 & , \text{ if } x \notin \Omega^* \end{cases} \quad (2)$$

Considering the energy bilinear form

$$a(u, v) = \int_{\Omega} \sum_{i,j,k,l=1}^3 E_{ijkl} \varepsilon_{ij}(u) \varepsilon_{kl}(v) dx \quad (3)$$

with linearized strains

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad , i, j = 1, 2, 3 \quad (4)$$

and the load linear form

$$l(u) = \int_{\Omega} fu \, dx + \int_{\Gamma_i} tu \, ds \quad (5)$$

The optimisation problem considered here is defined as follows:

$$\min_{\eta^*(x_e), i=1, \dots, n} l(u) = \int_{\Omega} fu \, dx + \int_{\Gamma_i} tu \, ds \quad (6)$$

subjected to constraints:

$$(i) \int_{\Omega} \sum_{i,j,k,l=1}^3 \tilde{E}_{ijkl}(\eta(x)) \epsilon_{ij}(u(x)) \epsilon_{kl}(v(x)) dx = l(v) \quad \forall v \in U$$

$$(ii) 0 \leq \eta(x) \leq 1 \quad \forall x \in \Omega$$

$$(iii) \int_{\Omega} \eta(x) dx \leq Vol$$

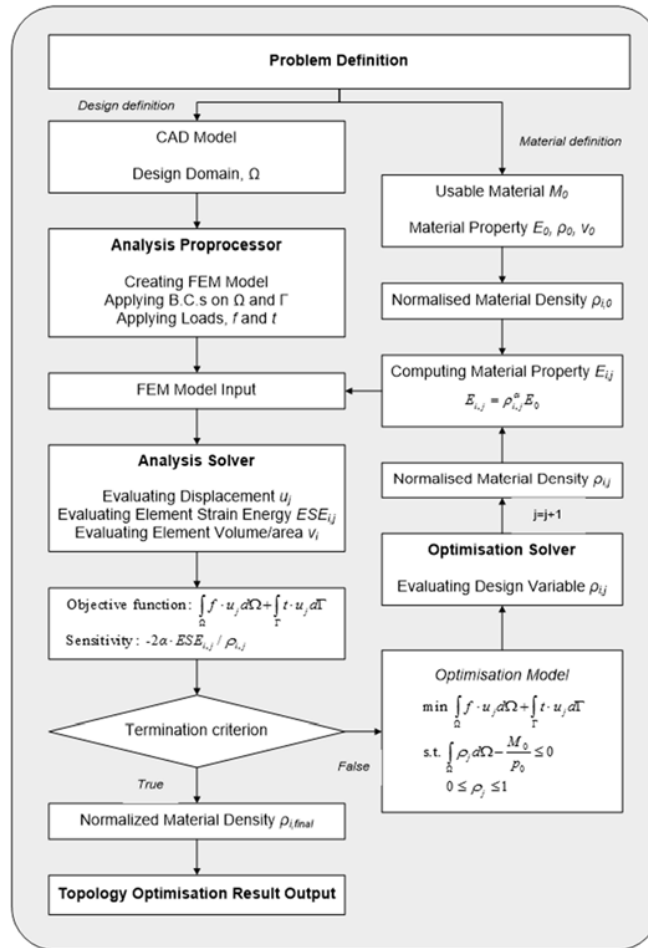


Fig. 1. A general topological optimisation process.

### 3. 3. Topological Results and Discussion

This approach is based on  $\mu$ CT data of real biological tissues to create the loading and constraint surfaces of the scaffold during the topological optimisation process. The goal of this approach is to obtain biomimetic optimised elements. In order to perform this kind of optimisation, a trabecular bone region was considered. The corresponding STL model is shown in figure 2. The STL file model obtained from the  $\mu$ CT data was analysed and non-valid triangles were removed and errors (overlapping, degenerated triangles, etc.) corrected. Once analysed and corrected, datum plane boundaries were created in order to define the scaffold element boundary space. The following step involves the intersection between the datum planes and the STL model to define the loading and constraint curves to define the surfaces for optimisation. The scaffold block element considered for the topological optimisations is indicated in figure 3.

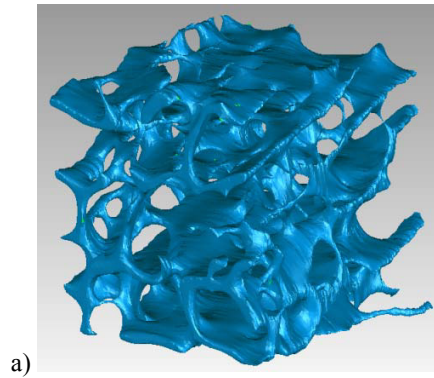


Fig. 2. a)  $\mu$ CT STL file after removing the triangular imperfections.

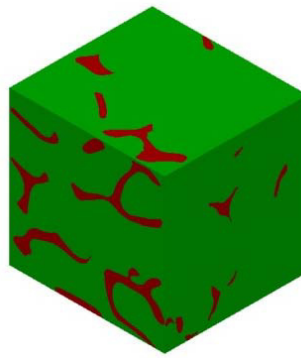


Fig. 3. Illustration of the scaffold block element considered for the topological simulations. Red – regions subjected to either loading or constraint conditions; Green – regions free of either loading or constraint conditions.

The porosity of the original  $\mu$ CT model within the STL file is 84 %, this was also the considered value for simulation purposes. The block element was assumed to have a linear elastic behaviour, so strain values of 0.1 were simulated by imposing a corresponding displacement according to the strain direction considered (0.2 mm along both X and Y directions, and 0.184 along the Z direction). A mesh of 98535 solid tetrahedral elements was used.

The following scenarios were considered (figure 4):

- Scenario 1: specific regions of the block faces were submitted to tensile stress in the XX direction ( $\epsilon_{xx}$ ) and a shear stress in the clockwise direction ( $\gamma_{yz}$ ) and the remaining specific regions were constrained (XX axis rotation).
- Scenario 1: specific regions of the block faces were submitted to tensile stress in the YY direction ( $\epsilon_{yy}$ ) and a shear stress in the clockwise direction ( $\gamma_{xz}$ ) and the remaining specific regions were constrained (YY axis rotation).
- Scenario 1: specific regions of the block faces were submitted to tensile stress in the ZZ direction ( $\epsilon_{zz}$ ) and a shear stress in the clockwise direction ( $\gamma_{xy}$ ) and the remaining specific regions were constrained (ZZ axis rotation).

In figure 4, the yellow regions are subjected to loading conditions while the blue regions are constraint regions. The grey regions are free of either loading or constraint conditions.

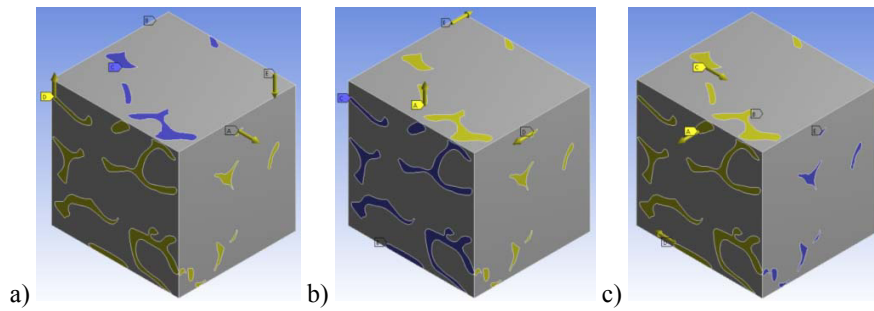


Fig. 4. Illustration the variation of the solicitations according to each direction: a) Tensile and Rotational Displacement in the XX direction b) Tensile and Rotational Displacement in the YY direction c) Tensile and Rotational Displacement in the ZZ direction.

The obtained results were:

- Scenario 1: Figure 5.a presents a valid topological scaffold model in 2 different positions.
- Scenario 2: Figure 5.b presents a valid topological scaffold model in 2 different positions.
- Scenario 3: Figure 5.c presents a valid topological scaffold model in 2 different positions.

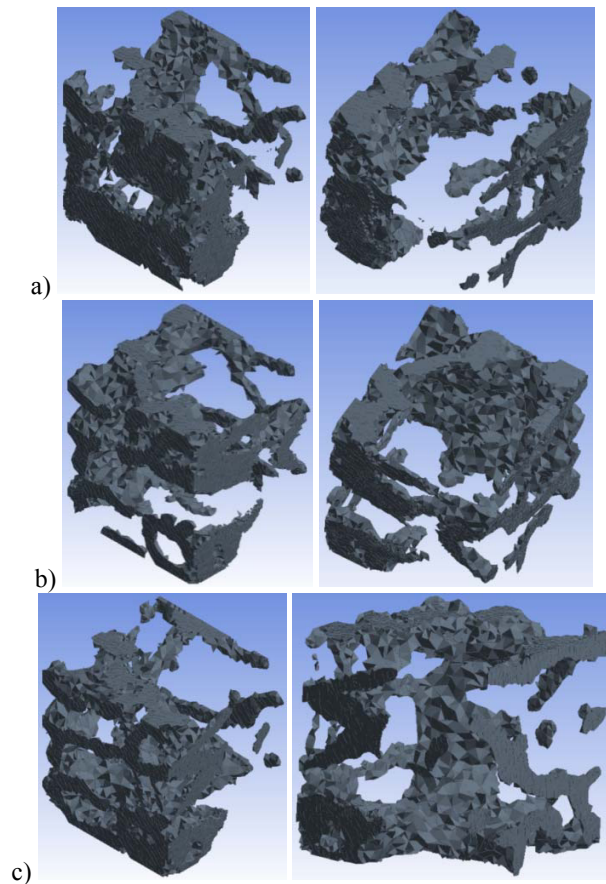


Fig.5. Illustration the topological optimisation results according to each displacement direction: a) DX - Displacement in the XX direction b) DY - Displacement in the YY direction c) DZ - Displacement in the ZZ direction.

Figure 5 illustrates the topological results for each case study. These results allow us to conclude that this approach enables to produce more biomimetic topologies. The initial external topology of the  $\mu$ CT data, which corresponds to a structure of a well-defined mechanical behaviour and porosity level is the starting point of an optimisation scheme that enables to obtain constructs with different levels of porosity and mechanical properties according to the required applications. The goal is not to obtain similar structures as the starting model, but instead to use the starting configuration to produce novel models with different characteristics but more biomimetic.

#### 4. Conclusions

Advanced additive manufacturing technologies, namely Biomanufacturing, are being used to fabricate scaffolds with controlled architecture for tissue engineering applications. These technologies combined with computer-aided design (CAD) enable to produce three-dimensional structures layer-by-layer in a multitude of biomaterials. Actual prediction of the effective mechanical properties of scaffolds produced by Biomanufacturing, is very important for tissue engineering applications.

One of the existing computer based techniques for scaffold design is topological optimisation. The goal of topological optimisation is to find the best use of material for a body that is subjected to either a single load or a multiple load distribution, maximising its mechanical behaviour under tensile and shear stress solicitations. The initial external topology of the  $\mu$ CT data, which corresponds to a structure of a well-defined mechanical behaviour and porosity level, is the starting point of an optimisation scheme that enables to obtain constructs with different levels of porosity and mechanical properties, according to the required applications, based on biomimetic external surfaces. This particular topological optimisation scheme uses the surface boundaries to produce novel models with different characteristics, which are different from the initial  $\mu$ CT models, enabling to design valid biomimetic scaffold topologies for tissue engineering applications.

#### Acknowledgements

The authors also wish to thank Prof. Anath Fischer from the Technion University in Haifa for supplying the Micro-CT data.

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