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POMES: An Open-Source Software Tool to Generate Porous/Roughness on Surfaces

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Abstract

The long-term success of implants depends on rapid healing and safe integration with body. In the case of orthopaedic and dental implants it was found that geometry and surface topography are crucial for short and long-term success of the implant, due to its effects in osseointegration. Properties of implant surfaces have been studied in the last decade in a concentrated effort to improve osseointegration process and implant success. Several researchers have proved that roughness of implant surface is related to healing time and integration between the implants and the bone, but the parameters on the surface creation are not fully controllable with current processes. In this work, computational algorithms are proposed for implant surface design in order to control the parameters required for this application. As a result it is presented an open-source software tool, called POMES - Porous and Modifications for Engineering Surfaces - , to design porous/roughness on top of surfaces in any geometry. Additionally, an example model was fabricated using POMES and additive manufacturing.

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1. Introduction

Osseointegration, defined as a direct structural and functional connection between ordered, living bone and the surface of a load-carrying implant, is critical for its stability, and is considered a prerequisite for its loading and long-term clinical success. A porous implant surface provides considerably more volume to promote cell attachment and bone tissue ingrowth, thereby facilitating a higher level of bone-implant interaction for cell migration and osteoblast adhesion into the implant surfaces [1]. This structural and functional union of the implant with living bone is strongly influenced by the surface properties of the implant. The performance of porous surface relies on a number of topographical features, including porosity, pore/particle size, pore orientation, etc [1]. Scientific researches assessing the influence of implant surface properties on bone healing have identified several factors which are important for osseointegration [2]. The surface characteristics of implant which influence the speed and strength of osseointegration include surface chemistry, topography, roughness, load, surface energy, crystal structure and crystallinity, chemical potential, among others.

According to Wennerberg et al.[3] and Shalabi et al.[4],

the roughness surface of implants is divided into macro, micro, and nano-roughness. The macro roughness comprises features in the range of millimetres to tens of microns. This scale directly relates to implant geometry, with threaded screw and macro porous surface treatments. The primarily implant fixation and long-term mechanical stability can be improved by an appropriate macro roughness. This will enhance the mechanical interlocking between the macro roughness features of the implant surface and the surrounding bone [3]. Micro roughness is defined as being in the range of 1 μm to 10 μm . This range of roughness maximizes the interlocking between mineralized bone and implant surface. Studies supported by some clinical evidences suggest that the micron-level surface topography results in greater accrual of bone at the implant surface [4,5]. Nanometre roughness plays an important role in the adsorption of proteins, adhesion of osteoblastic cells and thus the rate of osseointegration [6].

Some studies have demonstrated that there is a predominant relationship between the roughness surface of the implants in the osseointegration process. Wennerberg and Albrektsson[7] had shown that titanium implants with adequate roughness may influence its primary stability, enhance bone-to-implant contact, and may increase removal torque forces. According to Boyan et al.[8], the surface roughness of the implants can significantly change the process of osseointegration because the cells react differently to smooth and rough surfaces. Fibro-

blasts and epithelial cells adhere more strongly to smooth surfaces, whereas osteoblastic proliferation and collagen synthesis are increased on rough surfaces. Sammons et al.[9] and Zhao et al.[10] demonstrated that titanium surface roughness influences a number of events in the behaviour of cells in the osteoblastic lineage, including spreading and proliferation, differentiation, and protein synthesis.

A porous surface on titanium implants can be achieved by different manufacturing processes, such as grit-blasting, chemical etching, space holders, plasma spraying, among others. As it was shown by Guhenec et al.[11] and Liu et al.[12], these methods have drawbacks like low porosity, uncontrolled pore size and isolated pores by a lack of interconnection between them, being a problem for implant fabrication.

Also, several studies have shown that ceramic particle coatings based on calcium, like hydroxyapatite (HA), dicalcium phosphate dehydrate (DCPD), amorphous calcium phosphate (ACP) and others, enhance bone ingrowth and healing process. These coatings require an appropriated surface roughness in order to obtain mechanical retention of the coating and a good interface with the bone [11,13].

Computing systems are an important tool that can be used for the creation and design of controlled porous and roughness surfaces. Using computational design, mathematical algorithms can be used to create random and ordered structures that meet implant requirements and enhance their osseointegration properties. Given that, an open-source software tool was developed and proposed for implant surface design. This software is able to create and control rough and porous structures on the surface of any geometric model. The objective of this paper is to present this software and shows some preliminary results. The source code from POMES is available at <https://github.com/jcdinis/POMES>.

Additive manufacturing is a ground-breaking technology that supports the creation of any geometry based on the paradigm of layer-by-layer material deposition. Nowadays this is specially important because metallic biomaterials like titanium and its alloys can be used in additive manufacturing in form of micro-sized grain powder based and processed using a Laser Melting or Electron Beam Melting technologies to give form in final use parts. These processes can yield patient-specific prostheses production for final applications in medical and dental fields. Therefore, patient-specific prosthesis can be designed, based on medical imaging with an appropriate surface for osteointegration using POMES software, and then produced in additive manufacturing for final applications.

2. Methods

The software proposed in this paper allows for the creation of roughness and porous structures on the surface of any geometric model. The creation of these structures can be done in two ways. The first one is done by creating mathematical structures at any point of the surface taking into account the normal direction at this point, (see Algorithm 1). It is necessary to guarantee that the holes are in outside. The second way can be done through the creation of a shell around the solid mesh, and then generate rough structures randomly (see Algorithm 2).

The software proposed has a data base of roughness and porous structures, which are mainly composed of triply periodic

minimal structures. Such structures have the characteristics of growing in three orthogonal directions and a null average curve [14]. These periodic structure can be described by the following equation [9], [15].

$$\phi(r) = \sum_{k=1}^k A_k \cos \left[\frac{2\pi(h_k \cdot r)}{\lambda_k + p_k} \right] = C \quad (1)$$

Where r , represents the Euclidean vector space, and h_k is the reciprocal space vector, A_k is the magnitude factor, λ_k is the wavelength of the periods, p_k is the phase shift and C a constant. In the case of triple minimal periodic structures, the formulation of Weierstrass describes its parametric form [9]:

$$\begin{cases} x = Re \int_{\omega_0}^{\omega_1} e^{i\theta} (1 - \omega^2) R(\omega) d\omega \\ y = Im \int_{\omega_0}^{\omega_1} e^{i\theta} (1 + \omega^2) R(\omega) d\omega \\ z = -Re \int_{\omega_0}^{\omega_1} e^{i\theta} (2\omega) R(\omega) d\omega \end{cases} \quad (2)$$

Where the ω is complex variable, θ is designated as the angle of Bonnet and $R(\omega)$ is a function of the desired structure [9]. The data base of this software tool is composed by the following structures: Schwarz P (3), Schwarz D (4), Gyroid (5), Neovius (6) and W (iWP) (7):

$$\cos(x) + \cos(y) + \cos(z) = 0 \quad (3)$$

$$\begin{aligned} \sin(x) \sin(y) \sin(z) + \sin(x) \cos(y) \cos(z) + \\ \cos(x) \sin(y) \cos(z) + \cos(x) \cos(y) \sin(z) = 0 \end{aligned} \quad (4)$$

$$\cos(x) \sin(y) + \cos(y) \sin(z) + \cos(z) \sin(x) = 0 \quad (5)$$

$$3[\cos(x) + \cos(y) + \cos(z)] + 4\cos(x) \cos(y) \cos(z) = 0 \quad (6)$$

$$\begin{aligned} \cos(x) \cos(y) + \cos(y) \cos(z) + \\ \cos(z) \cos(x) - \cos(x) \cos(y) \cos(z) = 0 \end{aligned} \quad (7)$$

This software was developed using Python programming language, following the algorithms 1 and 2. The libraries used to develop this software tool were VTK (Visualization Toolkit - Kitware), Scipy and Numpy. The Figure 1 shows interface software tool. The surface generation is the implementation of these two algorithms:

```

input : Mesh  $M$ 
input : Function  $f$  chosen by user
output: Rough Mesh  $\hat{M}$ 
for each vertex  $v_i$  from  $M$  do
     $n_i = \text{normal}(v_i)$ ;
     $s_i = f(v_i)$ ;
    Orients  $s_i$  according to  $n_i$ ;
    Add  $s_i$  to  $\hat{M}$ ;
end
    
```

Algorithm 1: Rough surface by vertex

After the generation of the rough surface on the solid mesh. It is possible to export the 3D model in STL format to be produced in any additive manufacturing system.

3. Result and Discussion

A 3D model of an acetabular component was used to show the results of the developed software. As shown in figure 1, the user can select a surface rough structure and its parameters. After the generation, the user has a visualization of the resulting model. The figure 2 shows the result achieved by using the Schwarz P with 12 elements for each structure. As shown in the detail of the figure 2 the structures are distributed along the surface and the holes are directed to the outside of the surface. In the figure 3 it is possible to see how well the structures are assembled along the surface of the given model.

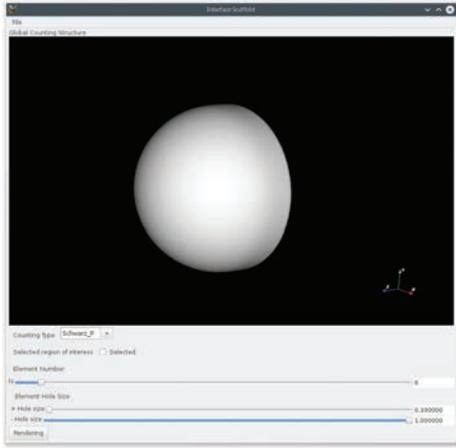


Figure 1. Software Interface

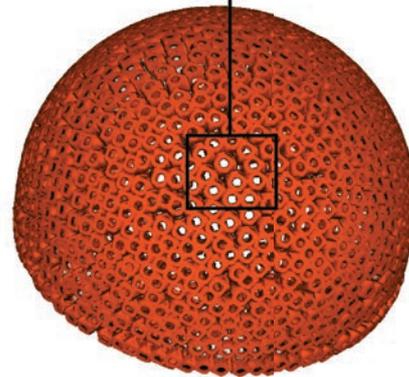
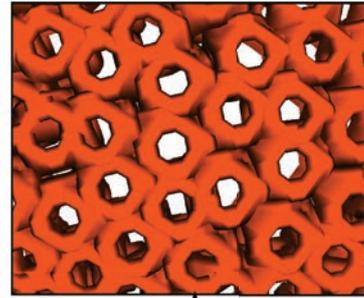


Figure 2. Schwarz rough surface obtained with structures P

```

input : Mesh  $M$ 
input : Function  $f$  chosen by user
output: Rough Mesh  $\hat{M}$ 
 $V = \text{voxelization}(M)$ ;
 $D = \text{dilation}(V)$ ;
 $C = D - V$ ;
 $H = C$ ;
for each voxel  $v_i$  from  $C$  and  $h_i$  from  $H$  do
    |  $h_i = f(v_i + \text{random}())$ ;
end
 $\hat{M} = \text{MarchingCubes}(H)$ ;
Algorithm 2: Rough surface by voxelization
    
```



Figure 3. STL model with Rough surface

It is possible to control the density of structures along the surface of the model by means of the parameter choice. The figure 4 shows a model with low density of rough structures and 9 element for each structure.

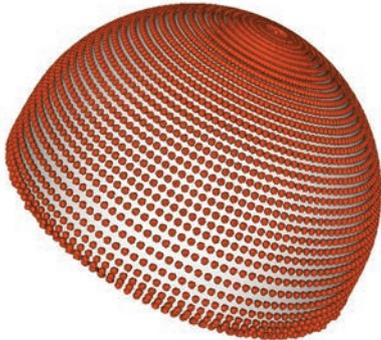


Figure 4. Model with lower density of roughness

The figure 5 shows the result obtained by the creation of a shell around the solid mesh, and then create rough structures randomly within that shell. The result presents a high variation of the size of pores and roughs. This technique is not able to control the surface roughness in a particular object region. Figure 6 presents a cutting of the resulting mesh showing the inside of the roughness surface.

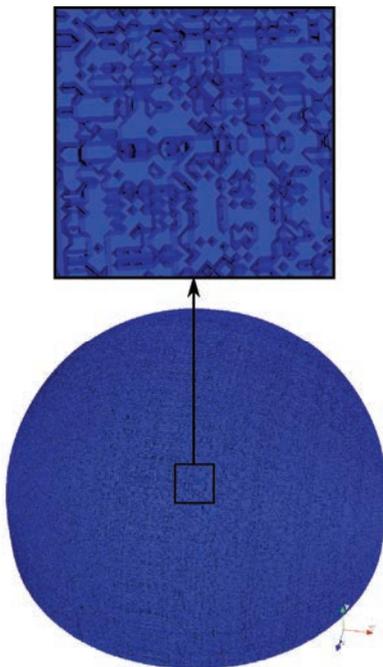


Figure 5. Roughness obtained randomly

The process can generate a very dense mesh, with a high number of elements. To reduce the number of elements, the vtk-DecimatePro filter, from VTK, was used. This filter implements

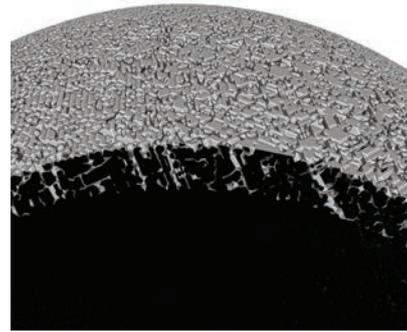


Figure 6. The STL model cut

the method described by Schroeder et al.[16], which reduces the number of triangles from a mesh with little loss of accuracy. This is necessary because the current additive manufacturing machines do not support very dense meshes. After designing the solid models with different rough surfaces and levels of porosity, the models were then produced on a CONNEX 350 from OBJET. This equipment uses the POLYJET technology and works with photosensitive resin materials called FullCure 720. Figure 7 shows the final object produced by this machine.

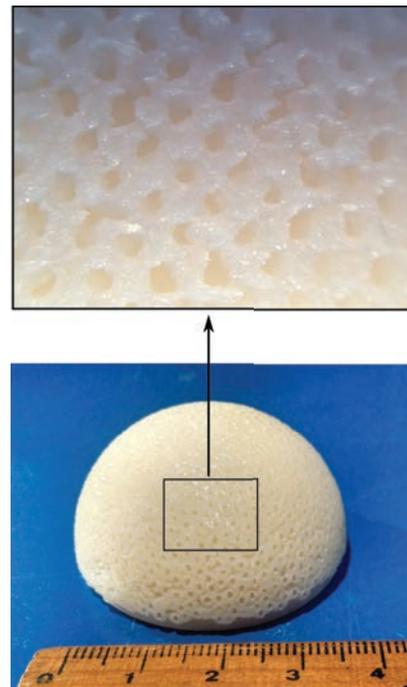


Figure 7. Manufactured object

4. Conclusion and Future Works

Advanced additive manufacturing technologies, including Biomanufacturing, allied to this software allows for the production of objects with porous and roughness structures. This inter-

action potentially permits medical applications, such as arthroplasty to promote rapid osseointegration between the prosthesis and bone. The software can produce any geometry, and place a rough constructed structure on surface of the region of interest. It can be seen in the above figures, that can be controlled the density of the desired surface roughness. The results were very satisfactory, producing a geometry model with high variation of porosity of the surface.

As a future work, it is intended that user to be able to use their own functions to generate the roughness. These processes can yield patient-specific prostheses production to find application in medical fields. Therefore, patient-specific prosthesis can be designed, based on medical imaging with an appropriate surface for osteointegration using POMES software and then being produced and applied.

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