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HETEROGENEOUS MATERIALS BASED ON APERIODIC STRUCTURES FOR BONE TISSUE SUBSTITUTES

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Abstract. Need for new materials with high porosity and thus low weight and also exhibiting high strength and suited to the requirements of specific applications stiffness gave direction to many studies towards an in-depth analysis of the microstructure of porous materials. Most frequently materials of this type require an adequate balance between parameters determining the mechanical and thermal properties and weight or porosity. The materials are applicable in the automotive, aerospace, production of the biomedical materials, power generation and chemical industry, also serve as insulating materials, energy absorbers (eg. on collision) as well as filters and strainers. High potential for the design of porous materials with a very wide range of properties justifies an interest in further research and development of new possibilities in manufacturing. In the medical field porous materials are often considered as the most suitable substitutes for bone tissue due to their lightness and strength. Demand from medical sector for materials of this type is continuously increasing while traditional methods of manufacturing of porous materials based on foamed metals, polymers, or ceramics are under development. The Advanced techniques for the preparation of porous structures based on 3D printing are becoming increasingly important with the development of rapid prototyping technology. Application of 3D printing also opens up new opportunities in designing and study the properties of more complex materials for medical applications with well-defined parameters of structures that are impossible to achieve using existing methods. So far, designed and manufactured by the 3D printing porous materials intended to be substitutes for bone tissue are generated mostly by duplicating one or more basic patterns. As a result, they have a periodic structure [1]. In this paper the fully analytical methods based on generating random graphs for point clouds are used for modeling structures [2]. Obtained in this way heterogeneous structures imitating the properties of bone tissue can be a potentially interesting alternative for materials produced using traditional methods. The structures obtained this way are aperiodic and may exhibit strong structural inhomogeneity. Studies presented in the paper show opportunities of modeling materials with given parameters based on aperiodic structures, as well as the prediction of their properties.

1 MODELING STRUCTURES

1.1 Point clouds generation

For topological modeling of a heterogeneous aperiodic material we use two different approaches. The first approach was based on application of hyperunifom distribution of points for generating nodes of trabecular network. The advantage of this solution is that resulting structure is fully aperiodic and isotropic. Another approach was to use spatial points distributions exhibiting three dimensional quasicrystaline ordering. 3d Amman grid which results from a special decoration of Penrose tilings can be projected from higher-dimensional crystalline structures they can be considered a case in between crystalline and amorphous. We first adopted the protocol suggested by Florescu and coworkers to map a hyperuniform point pattern into tessellations for trabecular materials design. As a seed structure we use the centroid positions from a maximally randomly jammed assembly of spheres of the same diameter with a volume filling fraction of $\varphi = 0.64$. As shown by Torquato and coworkers such structures based on random close packing (RCP) indeed possess the hyperuniform long-range correlations and show structural isotropic properties.

1.2 Delaunay tessellation

Next we perform a 3D Delaunay tessellation of the spheres center positions. In this scheme tetrahedrons are formed in such a way that no sphere center is contained in the circumsphere of any tetra-hedron in the tessellation. The centers-of-mass of neighboring tetrahedrons are then connected resulting in a 3D random tetrahedral network with the desired hyperuniform or quasicrystalline properties. Another solution was to build a 3D Voronoi diagrams for Delaunay tetrahedralization of a random point clouds (DT) . The next step was to build a 3D network from the edges of the Voronoi cells . Networks obtained in this way are less regular , compared to networks that are built on centers of mass of neighboring tetrahedrons, which have constant coordination number equal to four (four struts for each node). For the Voronoi diagrams based 3d networks the number of struts for each node is random. So we decided to use the network based on the center of mass, as a starting point for modeling the structures exhibiting desired mechanical properties and morphology.

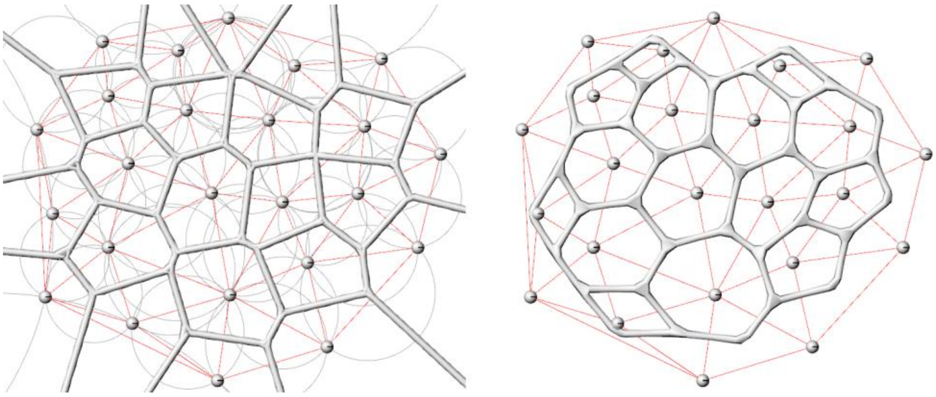

Figure 1: Construction of Voronoi (left) and Delaunay (right) tessellation

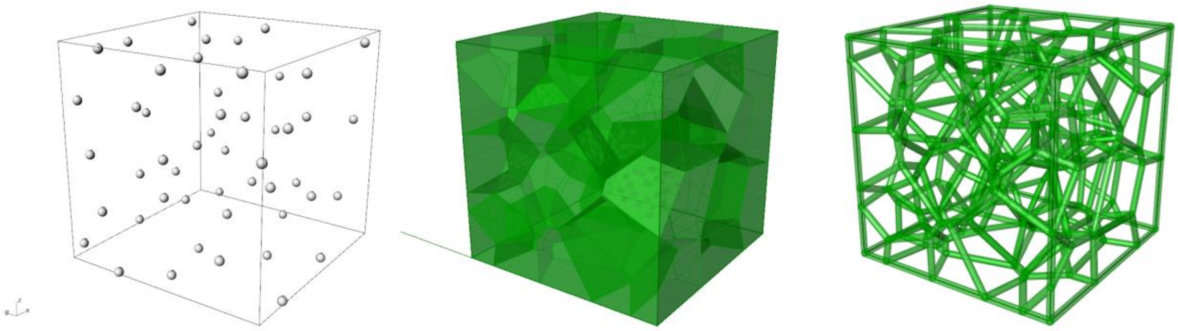

Figure 2: An exemplary method of obtaining the skeleton of the trabecular structure. From left to right: cloud points, the construction of Voronoi diagram, skeleton based upon the Voronoi cell edges

1.3 Trabacular structures

Both global and local properties of three dimensional network depend on trabecular thickness, length and number of connections. Trabecular structures with different properties were generated through thickening of struts between three-dimensional network nodes. Network of connections with a defined thickness has been transformed into a three dimensional surface, using computer-aided design software (CAD). The surface after optimizing has been saved in a standard stereolithography file format .stl. Prepared data can be directly used both in the preparation of input data for calculation using the finite element method and the preparation of input data for additive manufacturing.

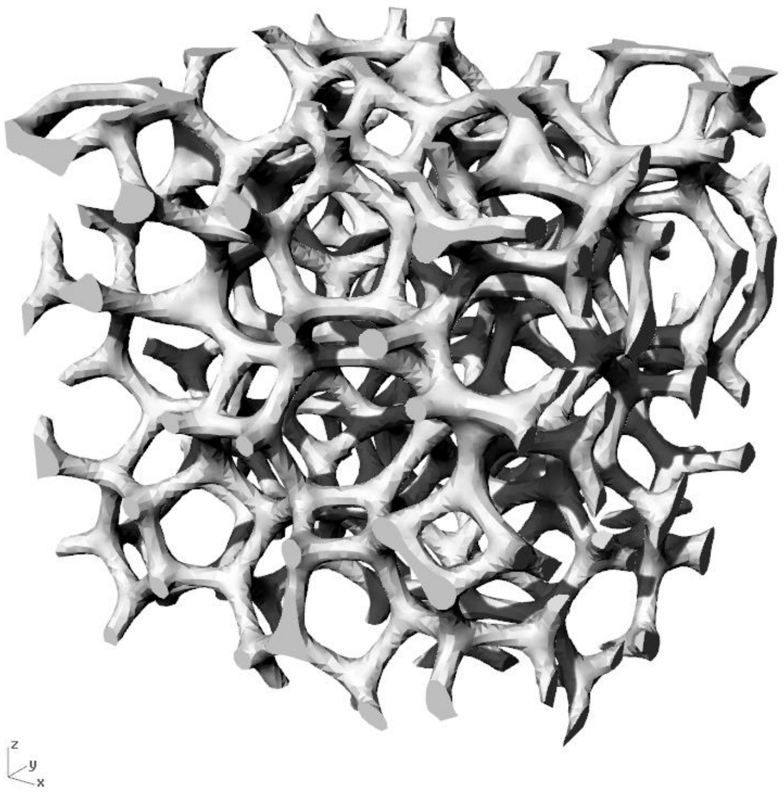

Figure 3: Optimized structure of the porous material, represented as a three-dimensional surface mesh. A fragment of structure, a box having a side of 5 mm used in the modeling of mechanical properties and test 3D printing.

1.4 Meshing of the generated and measured structures

One of the first step for the FEM analysis is decision whether the model will be one-, two- or three-dimensional, and then generation of the computational meshes. In the case of 3D structure, the model may consist of the first order elements, with two nodes corresponding to each edge or second order elements, with three nodes, including one lying on the center of the edge. Those elements are also referred to as linear and quadratic, which refers directly to a type of the related shape functions. The accuracy of the solution in the case of FEM can be improved by using a more dense mesh, the use of higher-order elements or the use of both these options. Most commonly a lower number of the higher-order elements allows to achieve the same level of the results accuracy as a greater number of the linear elements. Therefore, choosing the proper type of elements is crucial both for the sake of computational complexity, and hence the simulation time, as well as the memory load. A three-dimensional mesh generation for FEM, which consists of nodes and finite elements, is associated with a number of challenges, but allows accurately reflect the studied geometry. In the presented approach two methods of generating meshes will be used: directly from the voxel representation (voxel-based meshing) and through the intermediate step of the reconstruction of the surface (surface-based meshing) with the additional possibility of smoothing the structure. To generate a mesh from the surface reconstruction based on STL files (stereolitography), free and cross-platform gmsh software and library CGAL can be successfully used. They incorporate the best algorithms for the triangulation process, and also proprietary solutions, allowing to generate and export a mesh using INP format for FEM. By using these tools it is possible also to pre-test the quality of the mesh, change the order of the elements and read off the basic information about the generated meshes.

1.5 Modeling of the mechanical properties using FEM

Mechanical properties of the generated and manufactured structures were verified using Finite Element Method (FEM). Numerical simulations were performed to determine the global mechanical behavior of the whole structure based on the generalized Hooke's law that relates the stress to the strain tensor. Determination of the linear elastic constants constituting the fourth-rank stiffness tensor for orthotropic symmetry requires knowledge of nine material constants: Young's moduli for three orthogonal directions, three Poisson's ratios and three shear moduli. In the case of boundary conditions for such computational tests, there are two approaches: applying forces or displacements. For porous structures with complex topologies, the second is the most commonly used approach [8], and therefore it will be used in the case of computations for such structures. The results of simulations will be compared with the mechanical tests performed during the CT measurements on a miniature load machine. Experimental determination of the full tensor of elastic constants is very difficult. In particular the most problematic is the determination of shear moduli, especially in highly porous material. Due to the small dimensions and the difficulties in mounting a low volume porous materials, it is difficult to obtain strain state of pure shear. For that reason, true values of these parameters rarely appear in the literature. Thus, shear modulus will be determined indirectly by FEM simulations consistent with the experimental values for the remaining data (Young's moduli, Poisson's ratios). Typical boundary conditions for pure shear state (with given uniform displacements of specific model's nodes) effects in overstating values for the shear moduli, and the results are not fully consistent with orthotropic symmetry for structure. Therefore Mixed Uniform Boundary Conditions (MUBC) will be applied in order to minimize this negative effect [8].

Computer-aided study of the mechanical properties of the generated structures – numerical simulations were performed to determine the properties of the computer-generated structures. This will allow to selection of the structures with properties close to expected values, e.g. for anisotropy.

Table 1: Example of the stiffness matrix from FEM. Effect of extent of the box (i.e. number of nodes in the material), on the results of simulation. It can be clearly seen that for a box of size 9.5mm size effect vanishes.

5mm - stiffness matrix

1432	769,7	799,5	25,19	-4,451	-26,72
769,7	1389	767,7	12,72	3,911	-4,906
799,5	767,7	1369	25,7	-3,802	-8,861

39,09	42,41	39,99	279,6	-14,17	3,828
-13,55	-9,55	-17,47	-9,908	280,4	25,47
5,476	26,66	7,377	-3,236	17,68	258,9

9.5mm - stiffness matrix

1478	870,3	856,6	-4,811	1,114	2,488
870,3	1516	872,1	-7,567	-1,781	8,347
856,6	872,1	1484	-4,752	-5,446	7,27
-4,767	-8,865	1,367	302,8	1,911	0,08808
-0,852	-3,845	-8,467	1,384	295,7	-3,983
5,788	12,6	9,655	-1,06	-5,149	300,4

Table 2: Comparison of simmulated Young's moduli, Poisson's ratios and shear moduli for three orthogonal directions.

Box size	5mm	6mm	7mm	8mm	9.5mm
E_1 [MPa]	856,52	858,82	864,24	861,99	848,99
E_2 [MPa]	851,08	828,43	851,86	839,19	866,59
E_3 [MPa]	805,21	887,12	900,65	871,77	852,67
G_23 [MPa]	278,34	296,16	305,01	292,76	302,78
G_13 [MPa]	278,16	314,82	314	289,48	295,55
G_12 [MPa]	257,22	302,14	304,6	275,43	300,3
nu_23	0,36505	0,34549	0,36406	0,36629	0,37209
nu_13	0,39504	0,36298	0,35647	0,36162	0,36248
nu_12	0,33544	0,37217	0,37069	0,37	0,3655

1.6 Additive Manufacturing (AM).

To produce biocompatible porous structures of artificially generated bone-like models in meso- and macro-scale several AM methods were chosen. For each standardized input data in the form of STL files with 3D geometry of the structure were used. Fused Filament Fabrication (FFF) is AM method that uses a plastic filament unwounded from a coil to lay down material in layers and produce a part in analogues way to Fused Deposition modeling (FDM). Digital Light Processing (DLP) is AM method that uses a similar process to Stereolithography (SLA) with selective polymerization of model layers in liquid resins with the usage of light source. Selective Laser Sintering (SLS) is AM method that uses a laser as the power source to sinter powdered material to create a solid structure. Selective laser melting (SLM) uses a comparable concept, but in SLM the material is fully melted rather than sintered. Artificially generated 3D heterogeneous porous structures were manufactured in meso-scale resulting in cubic size of 5 mm using SLM (titanium alloy powder) and DLP (proprietary resin). High-resolution μCT measurements of the structures were performed after manufacturing.

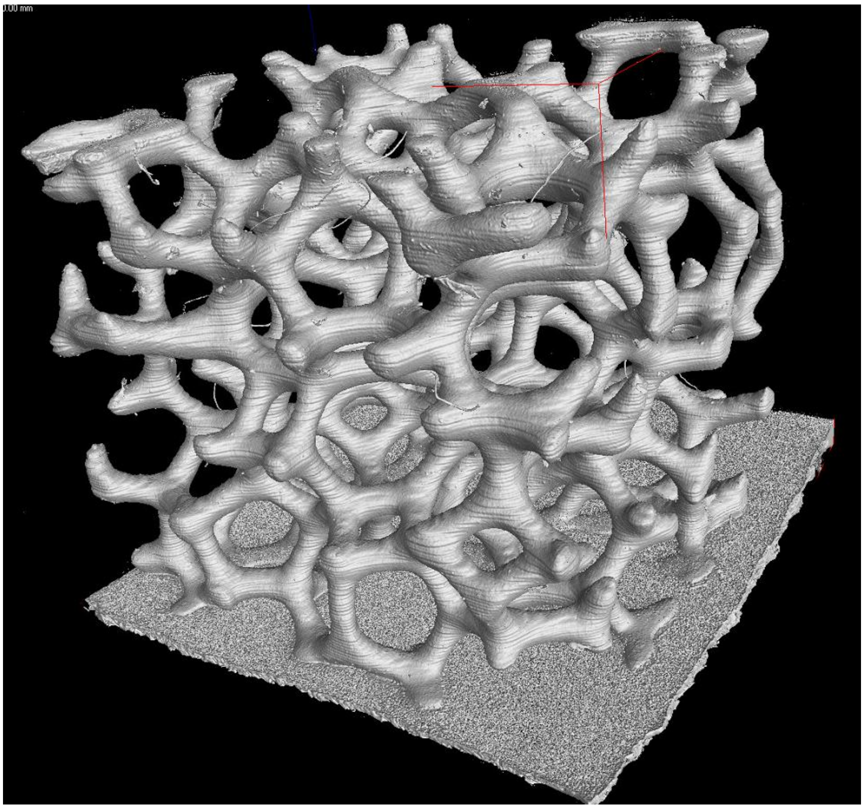

Figure 4: 3D heterogeneous porous structure manufactured using Digital Light Processing (DLP) technique in polymer resin. 3D reconstruction from X-ray microtomography (μCT).

1.7 X-ray microtomography (μCT) measurements

X-ray microtomography (μCT) is commonly known as a gold standard for evaluation of bone morphology and microarchitecture. It is also being used to study the porous artificial bone replacement structures. The use of μCT measurements allowed for the acquisition of the 3D structure and inspection of the surface roughness. It also provided the opportunity to use direct three-dimensional methods for the calculation of the morphometrical parameters such as porosity, diameters for the rods and pores, and the degree of anisotropy. Meso-scale artificially generated structures were measured in μCT with voxel size of 3.5 μm and also tested in miniature loading machine in linear range. FEM mechanical tests before and after manufacturing were also performed, allowing for the comparative analyses and positive verification of the whole process. The methodology can be illustrated based on the comparison of the input and prepared for AM methods geometries with the reconstructions from μCT scans. These results imply that DLP is currently the most suitable AM method in presented methodology, allowing for the exact reproduction of the geometry and properties of structure both for meso- and macro-scale. Further research may lead to strengthen the mechanical properties, which are actually too small in compare to bone tissue. Designing of the biomaterials paying special attention to fabrication of the geometry of porous structures shall be currently prioritized.

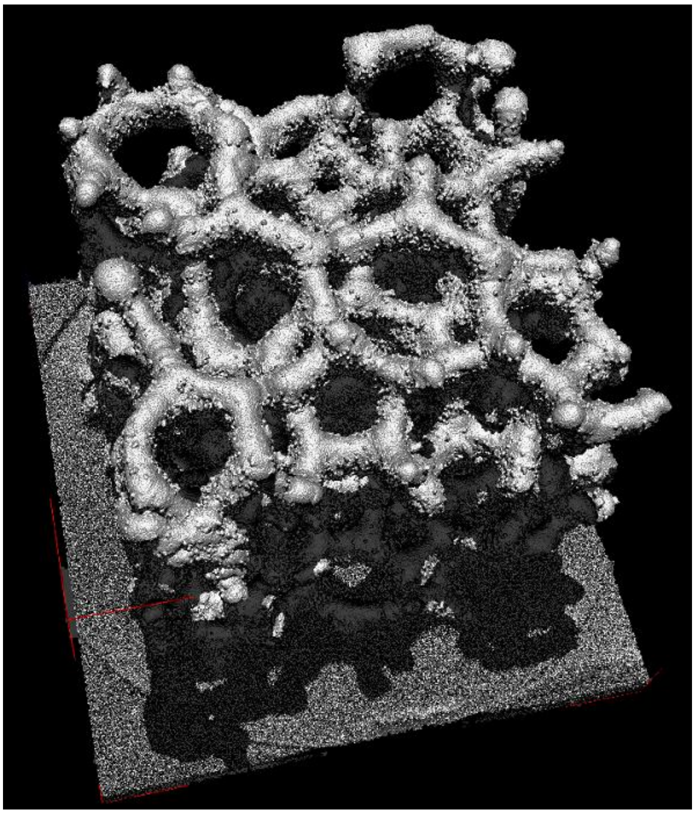

Figure 5: 3D heterogeneous porous structure manufactured using Selective laser melting (SLM) technique in titanium alloy. 3D reconstruction from X-ray microtomography (μCT).

Table 3: Morphology parameters (porosity [1 - BV/TV] , trabecular thickness) taken from ImageJ volume analysis of model strukture, DLP stack with slices of 30 microns resolution, DLP polymer resin 3D print, SLM titanium alloy 3D print.

ImageJ	BV/TV	Tb.Th.Mean [mm]	Tb.Th.Std	Tb.Th.Max	Tb.Sp.Mean [mm]	Tb.Sp.Std	Tb.Sp.Max

Model	0,08	0,243	0,049	0,319	1,466	0,235	1,764
DLP_slices	0,08	0,231	0,051	0,324	1,414	0,261	1,747
DLP_uCT	0,137	0,296	0,086	0,402	1,242	0,305	1,804
SLM_uCT	0,144	0,309	0,095	0,457	1,352	0,553	3,228

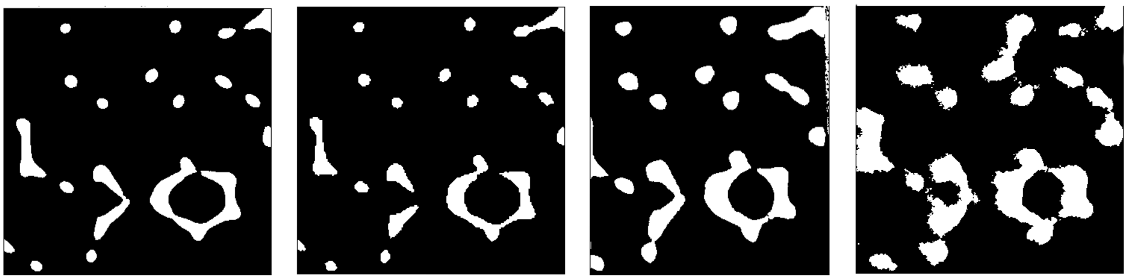

Figure 6: Comparison of the same slice taken from (from left to right) volume of model structure, DLP stack with slices of 30 microns resolution, DLP polymer resin 3D print, SLM titanium alloy 3D print.

2 CONCLUSIONS

The properties of aperiodic structures may change smoothly giving a big potential for systems with the required characteristics. Generating inhomogeneous aperiodic structures begins with the preparation of an appropriate set of points (called point cloud) in Euclidean space that meet certain order parameters. With simulation of rigid spheres homogeneous packing, taking point coordinates as sphere centers, depending upon the packing density can be achieved smoothly structure extending from the periodic arrangement of the FCC structure, maximum random packing RCP (random close-packing) or MRJ (maximally random jammed), which has an interesting feature called super-homogeneity (hipperuniform structure). Another group of aperiodic distribution points comprising anisotropic structure may be generated by the projection of the multidimensional space. Thus prepared sets of points are used to generate the skeleton connections with the methods based on Delaunay triangulation or Voronoi diagrams. Choosing the right method and parameters makes it possible to control the generated topology structure considering the relevant parameters such as number of connections in the nodes, the angles between the edges and so on. By appropriate selection of bolding and shaping of each connection, based on the skeletal structure the trabecular hetero-structure is formed. Porosity and nature of trabeculae (plate-like, rode-like may be controlled. The next step is to generate the surface and volume meshes for testing the mechanical properties of 3D printing by FEM. The proposed approach makes it possible generated structures with smooth changes of density, porosity and shape of the connections in any direction. Thereby allowing relatively easy modeling of transition between areas of spongy and compact bone tissue. The proposed attempt allow also to faithfully reproduce a naturally irregular shape of the bone or to impose on the modeled structure a specific bone tissue density maps. When you create a model of inhomogeneous structures, in addition to complying with the morphological and topological parameters of the bone also the technical possibilities of 3D printing techniques are taken into account (like voxel size, geometric constraints limitations, the possibility of the use different materials - in our case photopolymers and titanium).

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