Particle-Packaging Methods for Computational Modeling of Bones

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Abstract: Modeling the geometry and behavior of human bones is of the most concern when dealing with bone remodelling (external and internal) and poroelastic analysis. Complex geometries are frequently found in the human skeleton as well as orthotropic behavior of bone tissue. Spongy bone has a completely different constitution as compared with compact bone, which adds another relevant consideration if we want to get reliable results in biomechanical analysis. The modeling of both compact and spongy human-bone tissue is carried out by using packaging-particle methods. The methods generate circles (2D domains) and spheres (3D domains) in a random manner for the representation of non homogeneous and porous media. These methods were optimized with front-advance algorithms, which lead to a significant reduction of the very large set of circles and spheres. The methods use non-spherical particles (ellipsoids) to represent spongy bone. Some preliminary models of human bones are discussed.

Keywords: particles, packaging methods, biomechanics modeling, spongy bone, compact bone

1   Introduction

Several procedures to generate volumes formed by different types of particles can be found in technical literature. Feng *et al.* (2002, 2003) discuss an efficient and simple algorithm, which can be easily extended to other 2D particles. The authors present a good survey of the main methods and their basis. The key idea of Feng's work is to continuously update (in a dynamic manner) the particle-front surrounding all other particles. The updating of this front significantly reduces the amount of particles that must be considered in order when adding a new one. A local optimal

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density is then obtained and, as well, the packaging process is very fast. Also, the area can be further enlarged by a boundary compression and by using gravitational compaction, thus avoiding instabilities in some particles.

The extension of particle-packaging methods to 3D domains is not a trivial task. The same authors in other publication (Han *et al.*, 2005) proposed the extension from 2D to 3D. In this case, it is only needed to detect the intersection of two particles and to find the center of the new particle to be added, in order that it remains in contact with the previously found two particles. The ellipsoids packaging were also described by Wang and Liang (1997), who presented a front-advance algorithm, able to force the tangency between the new ellipse and the previous two. Wang *et al.*(1999) have extended this approach to 3D, although in this last case, the generation algorithm is somewhat slow. It is based on a kinematic scheme considering no-penetration of solid bodies. Ferrez (2001) discussed an interesting problem in industry: to determine the optimum proportion of particles having three different sizes in order to get a set of spheres with maximum density. This is a non-convex optimization problem, with quadratic restrictions and linear objective function.

Löhner and Oñate (2004) described another general method, also based in front-advancing techniques, to pack objects of arbitrary shapes. To get denser packaging, two procedures are discussed: a) to define closer objects during the generation and b) to move and to enlarge particles after the generation. The formulation is illustrated with ellipses, sphere collisions or near-sphere shape collisions. When the intersection of two particles is too complicated, it is recommended to represent the bodies by spheres. As well, the methods presented in this work are very efficient and general, since the procedures are suitable for several numerical methods, such as finite elements or distinct elements. One disadvantage of these methods is that control over the statistical distribution of particle dimensions may be lost during the particle enlargement phase.

Pérez *et al.* (2009) present another method and a computer code, able to pack several types of particles. The class-design implemented in this work allows the inclusion of any new particle type. The algorithm needs: a) a procedure to force the contact of the particle with other two particles (2D case) and three particles (3D case) and b) an intersection detection algorithm. The author reports some examples modeled by large sets of particles ($O(6)$ and $O(7)$), with speeds around 1000 particles/sec. The global volume fraction was over 51%. These authors also reported interesting results with direct applications to curves and surfaces as well.

There also exist generation schemes based on collective-rearrangement, such as discussed by Han *et al.* (2005). These authors developed an algorithm for the 3D packaging of spheres, which is easily adapted to other types of particles. The algorithm is based on a geometric idea of compression, by employing a neighbor efficient

search method (Perkins and Williams, 2001). The technique is to generate several layers of spheres which are compressed to fill the desired geometry. Another collective-rearrangement technique is based on particles-layer generation which is further compressed until an stable position is reached, by using the Conjugate-Gradient Method (CGM) as suggested by Nandakumar *et al.* (1999). Particle-packaging using spheres and non-convex polygons is presented in this work.

Maximum density is required in some practical applications. This can be achieved by formulating the packaging-particle problem as an optimization problem. Sutou and Dai (2002) worked with 3D packaging-particles (spheres) to fill the largest possible volume. This is a non-convex quadratic optimization problem with quadratic restrictions and linear objective function (some variables are real and some others are binary). It can also be shown, from a computational point of view, that the proposed algorithm is efficient.

Ferrez and Liebling (2002) have presented formulations to obtain particle packs with maximum density and low computational cost. This formulation is quite similar to the one presented in Sutou and Dai (2002), except that now all the variables are real. As well, some interesting problems related to particle-packaging are discussed. More recently, Siiriä and Yliruusi (2007) discussed the effects of friction, size and elasticity on the 3D packing of particles, showing that the higher the friction the smaller the packing density. Their approach was based on Newtonian mechanics. Jerier *et al* (2010) proposed a method to pack spherical particles using controlled overlaping. The particles are defined and created into a tetrahedral mesh, allowing to get very large scale packages.

The main goal of this paper is to introduce modifications to existing packaging algorithms in order to efficiently model very complex geometries such as those encountered in biomechanics and human tissue simulation.

2 Materials and Methods

2.1 *Particle-packaging methods*

Some particle-packaging algorithms are described in this work. For many applications, such as the Distinct Element Method (DEM), it is advisable that particles are as close as possible, each other. Figure 1 illustrates a classical example of particles modeling an irregular surface

Particle-packaging algorithms allowing up to 51% of volumen fraction (high density packs) are already developed and tested (Pérez *et al.*, 2009). The algorithm presented in this work is based on the front-advancing generation scheme of Feng *et al.* (2002), and is summarized into three main steps:
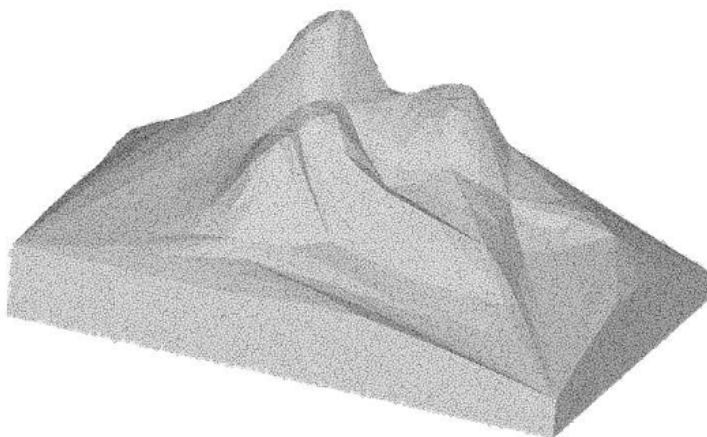
Figure 1: Model of irregular surface: 336344 particles

1. To create the new particle that will be added to the set of particles

2. Active front selection and determination of the new particle position, which will be in contact with other particles forming part of the front: one in the 2D case or two in the 3D case.

3. Check if the new particle intersects other particles already created. If no overlapping occurs then the new particle is "approved", continuing with the generation cycle until the volume is filled. Otherwise, the new particle position is rejected and step 2 is repeated until an active front is not found.

4. To illustrate the algorithm operation, a flow-chart is included below (see figure 2)

The procedure described above needs to hold an active-front, which is continuously updated either with each new particle or when finding a particle completely surrounded by others. This can be considered as a front-advancing scheme. C_{ext} is the active front whereas p_{piv} is the pivot-particle, representing this part of the front to grow immediately, since the new particle will be in contact with p_{piv} and one of its neighbors as well. Pérez *et al.* (2009) have implemented this procedure, also considering some variants of the method which lead to a different geometrical patterns and different degrees of efficiency. The main advantage is that high density packs can be generated, displaying a volume fraction of 51% and a particle generation speed of 1260 part/sec.
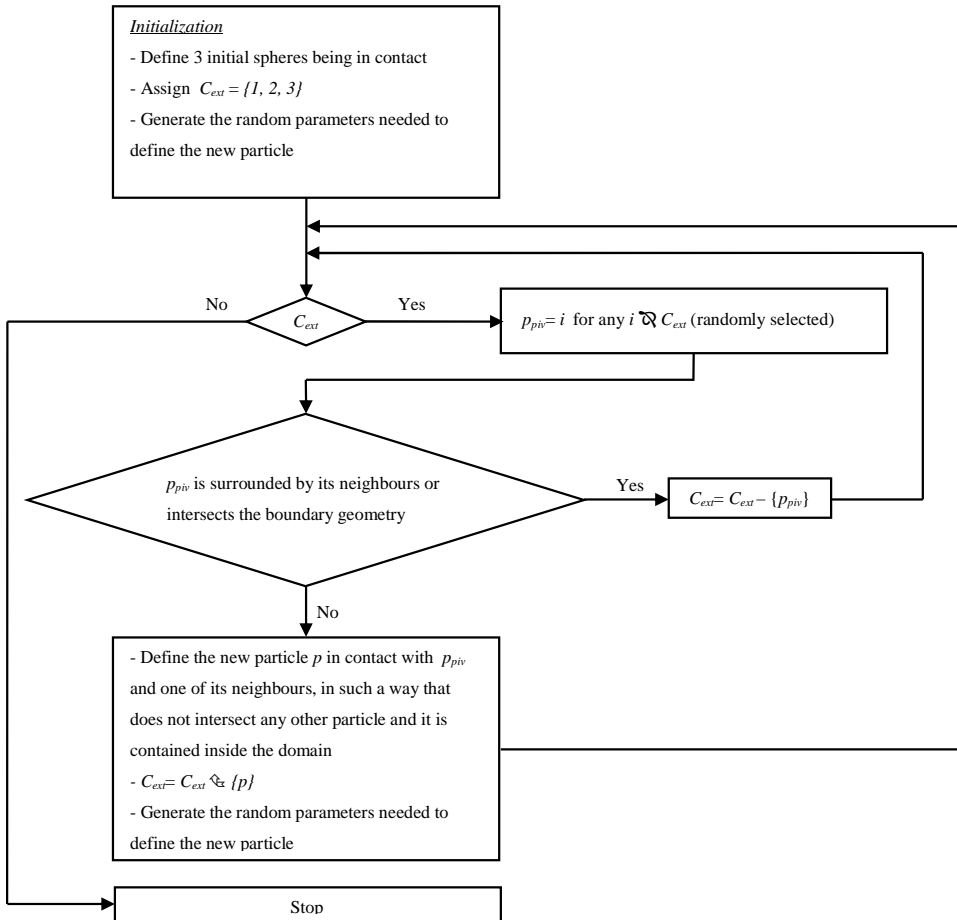
Figure 2: Flow-chart of particles-packaging proposed algorithm

In the described algorithm, the advancing-fronts has triplets of spheres not necessarily tangent each other. Other successful implemented variant includes a fourth sphere tangent to the previous three (similar as described in Feng et. al, 2002). This formulation gives average speeds over 3000 part/sec in most cases, and densities close to 50% for a U[1,2] distribution of the spheres radii. The advantage of the methods described in this section is that they allow the generation of high density packs but they are not able to reproduce the bone trabeculas (spongy bone). Thus, by introducing some modifications, we will be able to deal with complex geometries usually encountered when modeling human bones.

2.2   Geometric modeling of bone tissues

Spongy bone can be regarded as a continuum medium displaying elongated holes following the stress lines, i.e., an orthotropic material (see for instance Goldstein *et. al.,* 1991). This has been modeled, in this work, by using packages having either circular or spherical particles. The generated domain has elliptic holes with their main axis following a predetermined orientation. This research has developed several methods to get particle-packages forming elliptic holes (resembling the typical trabeculae organization). These holes are coated by a compact layer of particles, which can be used to model spongy bone surrounded by cortical bone. These methods are:

Method 1

Once a mesh of rectangles is superimposed to the particle pack, the ellipses are defined inside the rectangles (having their axes parallel to the rectangle sides) and then, the circles inside the ellipses are deleted. The ellipses can be defined by using a binary matrix whose terms are calculated either deterministically or randomly. For instance, see the figure 3 and its associated matrix.
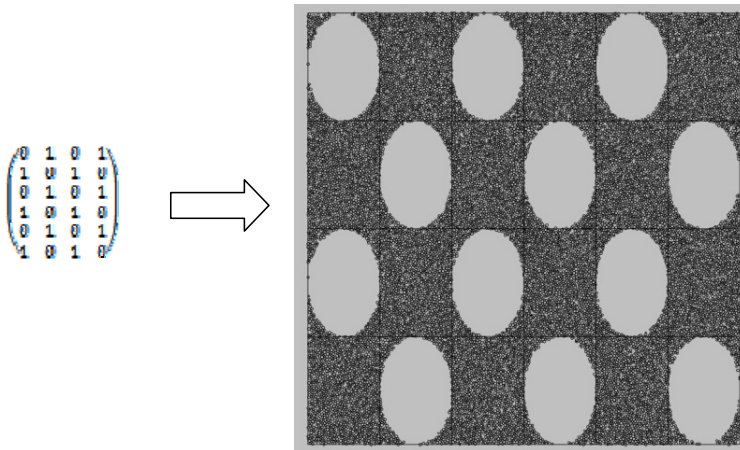

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

Figure 3: Uniform elliptic holes: matrix and graphic representation

Method 2

In this method, a large-size circles pack is superimposed over a small-size circles pack. Then, the small circles inside the ellipses defined by the large circles are deleted. As well, the ellipses has a small angle of inclination, defined randomly. In figure 4, a 600 units-side square has been filled with circles of distributed radii,
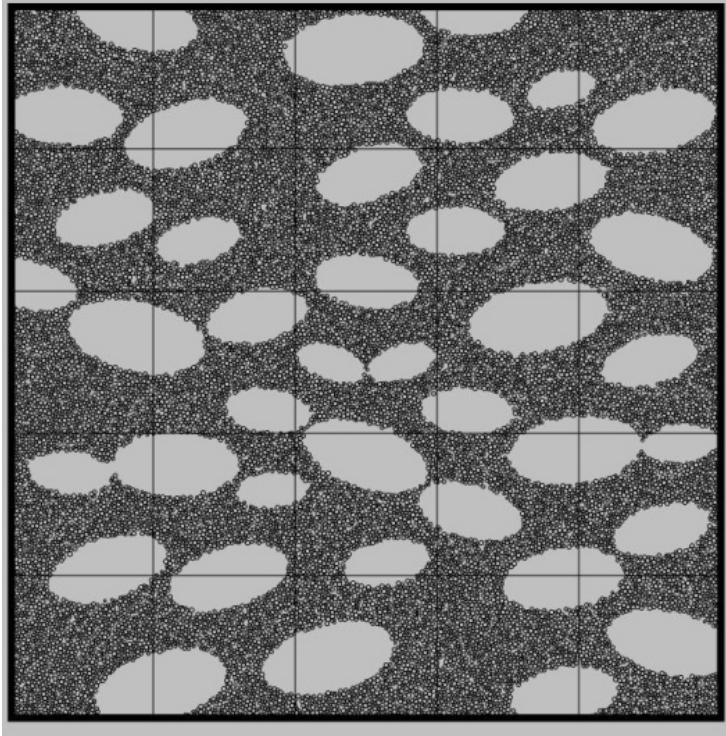
Figure 4: Random elliptic holes

following U[1,2]. The elliptic holes have been obtained from a circle package of distributed radii following U[30,60].

Method 3

A particle P_i is randomly selected. Then another particle is defined concentrically to P_i, having a radius randomly selected between the minimum and the maximum radii of the particle-packaging. The selection of P_i is carried out by generating a random number between one and the number of particles of the pack. The new circle P_k which is defined over P_i, will be centered at P_i and its radius follows a distribution whose maximum value (radius$_{max}$) and minimum value (radius$_{min}$) are calculated by

$$radius_{\max} = \frac{Rpart_{\max}}{D_r} \tag{1}$$

$$radius_{\min} = \frac{Rpart_{\min}}{D_r} \tag{2}$$

where $Rpart_{max}$ and $Rpart_{min}$ are the maximum and minimum particles radii and D_r (density relation) is the relation between the porous and the dense zone of the material being studied. In this manner, to compute the new radius (r'_k) a random number is generated, following the distribution $U[radius_{max}, radius_{min}]$, as shown in figure 5.
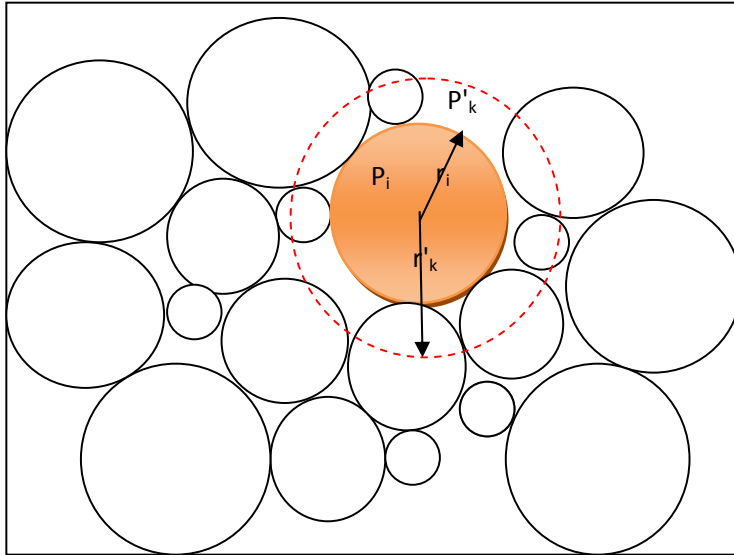

Figure 5: Concentric circle P_k over P_i

In the next step, all particles intersecting the new circle P'_k go again to previous step. This process is repeated until a predetermined quantity of the particles is deleted. This quantity is calculated by multiplying the total number of particles times the density relation. Two examples of particle-package are shown in figures 6 and 7.

Method 4

The radius threshold (R_t) is calculated from $Rpart_{max}$ and $Rpart_{min}$ and the density relation as follows:

$$R_t = Rpart_{max} - D_r * (Rpart_{max} - Rpart_{max}) \tag{3}$$

Then, all particles having a radius larger than R_t are deleted. Figures 8 and 9 display preliminary results obtained in this research. It can be observed that the algorithm allows the reduction of the density in an uniform way.
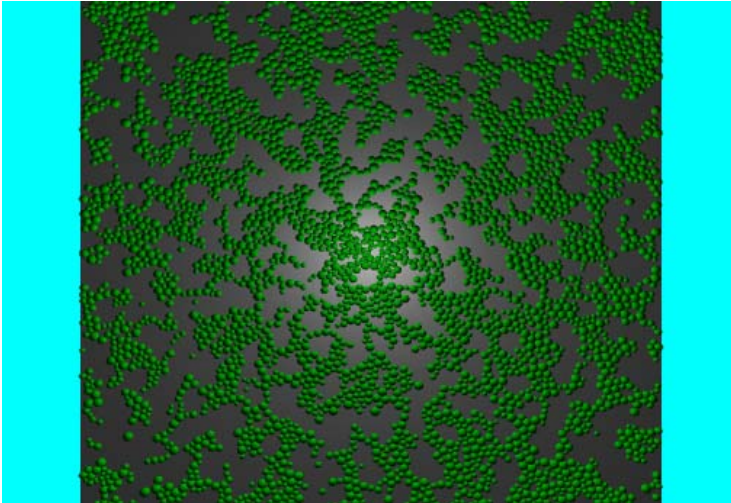
Method 5

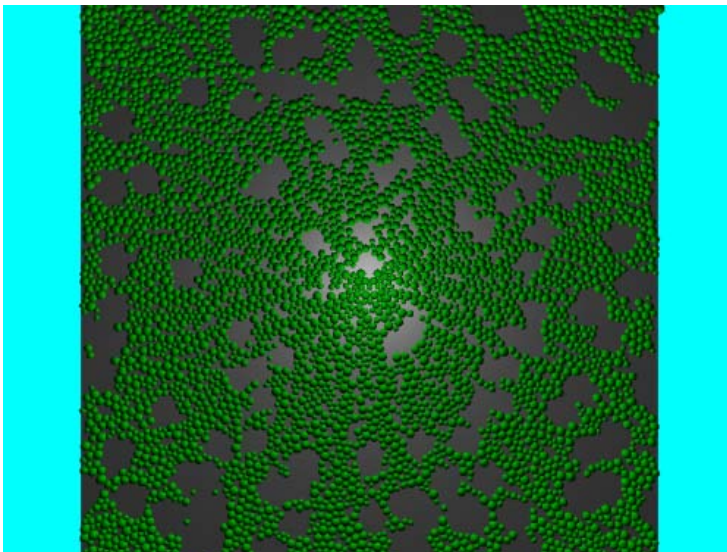Figure 6: Particle pack obtained with Rpart$_{max}$ =2.0 and Rpart$_{min}$ =1.0. D$_r$=0.5

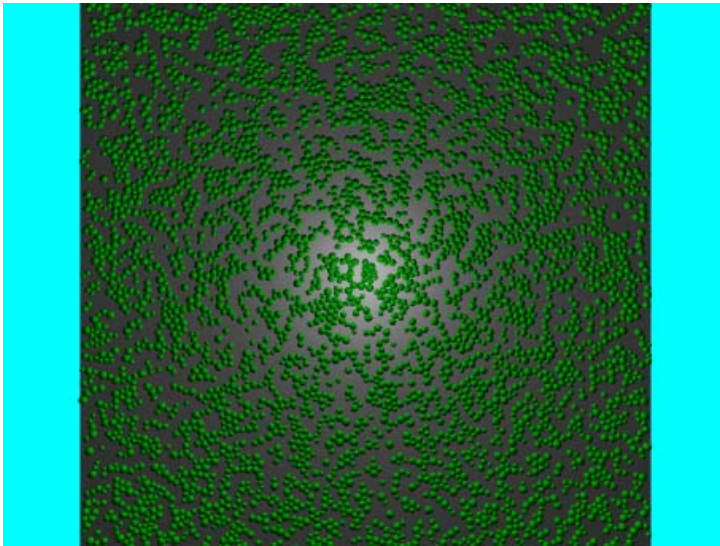Figure 7: Particle pack obtained with Rpart$_{max}$ =2.0 and Rpart$_{min}$ =1.0. D$_r$=0.3

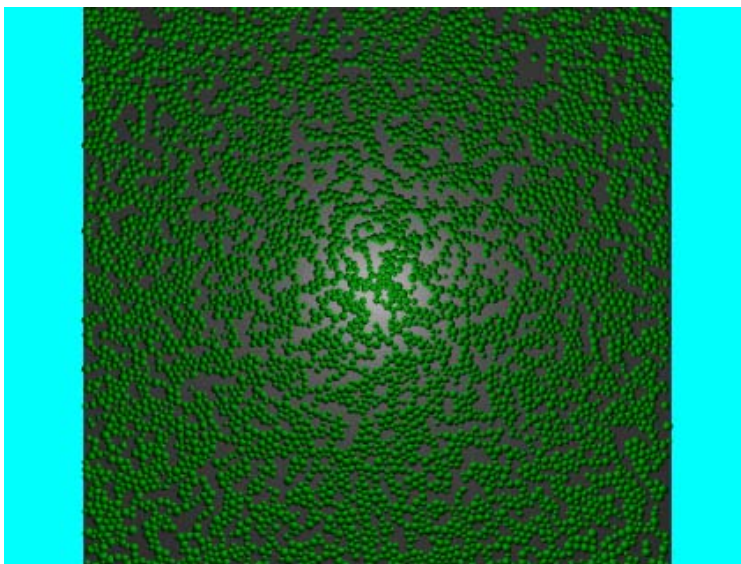Figure 8: Particle pack obtained with Rpart$_{max}$ =2.0 and Rpart$_{min}$ =1.0. D$_r$=0.3

Figure 9: Particle pack obtained with Rpart$_{max}$ =2.0 and Rpart$_{min}$ =1.0. D$_r$=0.15

The method proposed herein has been combined with a front-advancing technique. Although it is recommended to reduce the material density below a percentage value, it is not the best alternative for the problem discussed here. The method builds a particle-packaging, which representation involves circles treated as particles as well as circles treated as holes. In this sense, each type of elements (particles and holes) has its own distribution, and both will be built through the front-advancing method. Each advance-front can be formed by either two holes, two particles or by a particle and a hole. The geometric problem faced herein is the same as in the classical variants, except that now all circles representing holes will be deleted at the process end. To determine if the forthcoming element to be added will represent a particle or a hole, a probability value is associated to each element, having in mind that where P_{hole} is the probability that the circle is a hole and P_{part} is the $P_{hole} + P_{part} = 1$ probability that the circle is a particle. In this manner, by generating a random number between 0 and 1 and having the probability associated to one of these elements, it is possible to obtain porous packages with a front-advancing technique. Figures 10 and 11 illustrate two of these porous packages.
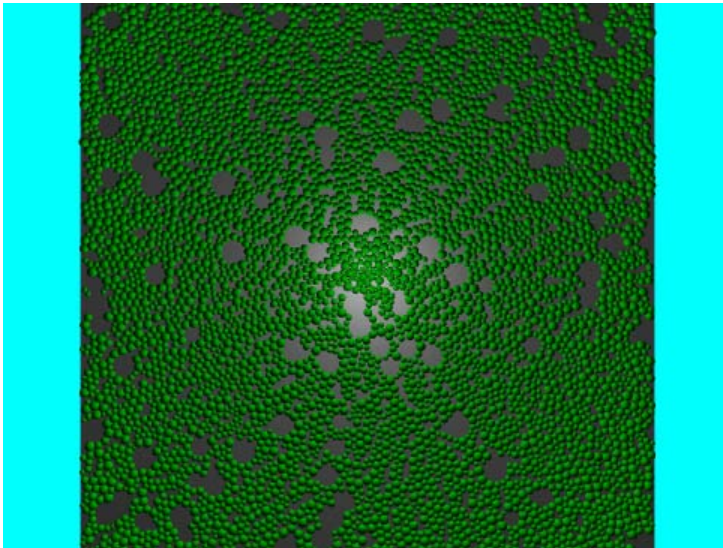

Figure 10: Porous package obtained: radius$_{hole}$ $\sim$U[3,5], radius$_{part}$ $\sim$U[1,2], P_{hole} =0.02

There exists a relationship between the probabilities of particles and holes and the final material density of the generated domain. To have some degree of control over
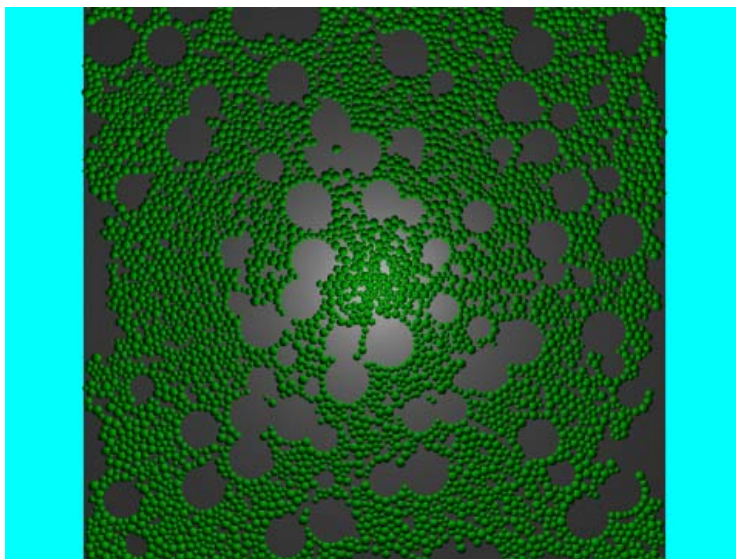
Figure 11: Porous package obtained: radius$_{hole}$ ∼U[3,10], radius$_{part}$ ∼U[1,2], P$_{hole}$ =0.02

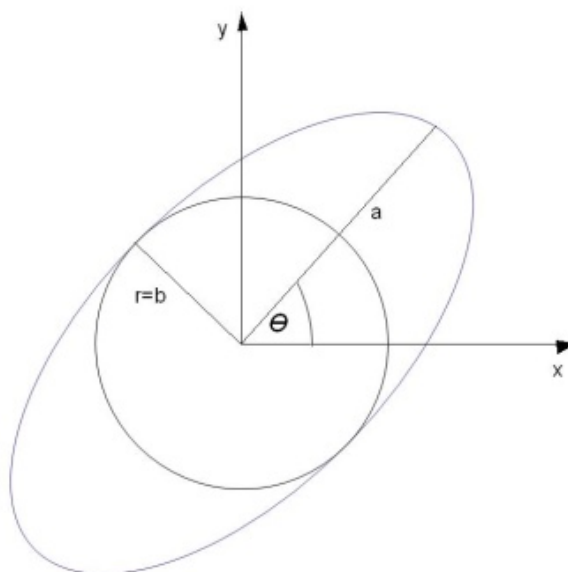Figure 12: Ellipse of axes a and b, circumscribed over a circle of radius b.

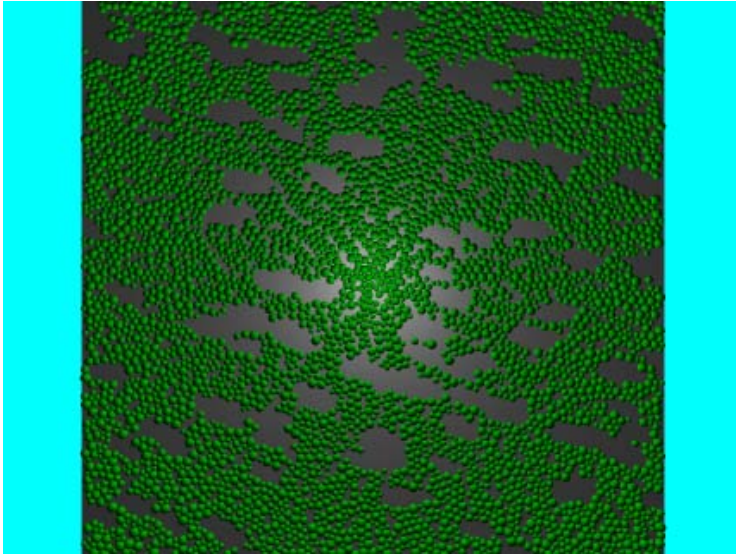Figure 13: Porous package obtained: radius$_{hole}$ $\sim$U[3,5], radius$_{part}$ $\sim$U[1,2], P$_{hole}$ =0.02, $\phi \sim U[0°, 30°]$

this relationship it is required to carry out a statistical study, which is beyond the objectives of this work.

Method 6

This method is an extension of method 5 and it is based on the apparent elliptic-shape associated to bone trabeculae, which has been modeled with ellipses inclined zero degrees. Circles representing the holes are generated inside the ellipses (see figure 12) and then, all particles having its center inside any of these ellipses are deleted, in such a way that elliptic holes remain into the circled-particles packaging.

As shown in figure 12, ellipses are circumscribed around large circles, being coincident the circle radius and the ellipse minor axis. Figures 13 and 14 show particle-packages obtained with method 6.

3 Results: Modeling of Human Bones

The already described methods have been extended to three-dimensional domains, by creating ellipsoidal voids in the particle-package. An ellipsoid can be represented by the parameters *{x_c, y_c, z_c, a, b, θ_z, θ_x}*, where x, y and z are the center coordinates, a and b are the ellipsoid axes (the two minor axes are similar) and θ_z, θ_x are the angles of inclination of the ellipsoid.
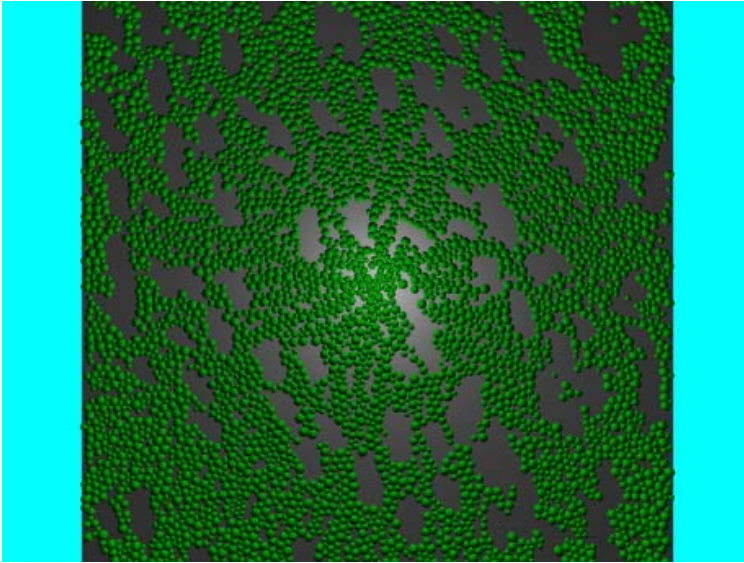
Figure 14: Porous package obtained: radius$_{hole}$ $\sim$U[3,5], radius$_{part}$ $\sim$U[1,2], P$_{hole}$ =0.02, $\phi \sim U[30°, 90°]$

To obtain the initial geometry a small cube was filled with spheres. Then, some spheres were removed thus leaving ellipsoidal holes where the distributions θ_z, θ_x were U[0, 2π] and U[-ε_z, ε_z] respectively, being ε_z=0.358. Figure 15 displays a thin slice of this cube. It can be noted in the figure that the external part has no holes and it works to model the cortical bone, whereas the internal part has elliptic holes, thus being suitable to model spongy bone. These aspects are of the most concern when dealing with internal and external bone remodeling (Cowin and Hegedus, 1976; Martínez and Cerrolaza, 2006; Martínez *et al.,* 2006) and poroelastic bone analysis (González *et al.,* 2009).

The algorithm proposed in this work is used to generate particle-packages for modeling three human bones: skull, hip and mandible. All of these bones have complex geometries. The three dimensional domains are first represented with a boundary element mesh and then modeled with the particle-packing algorithm, as shown in figures 16, 17 and 18.

Good results have been obtained, but however some aspects must be improved. For instance, it is mandatory to carry out extensive studies on the trabeculas shape, in order to model them in a better way. Other relevant subject is the CPU time for models generation. When the external boundary is not too complex, large sets of
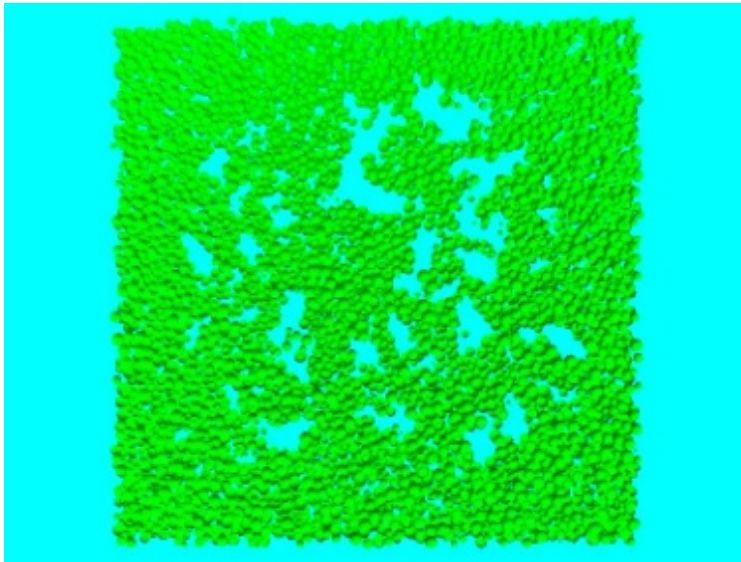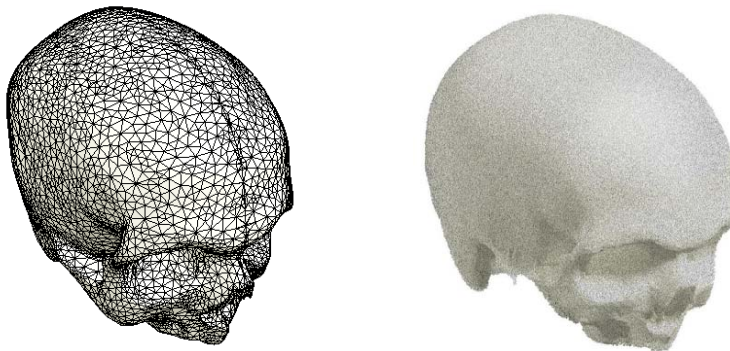
Figure 15: Extension to 3D of method 6

Figure 16: Human skull: a) boundary element mesh b) 1101921 particles model

particles can be obtained in a very efficient way. For instance, a simple cube is filled with 1931732 particles in approximately 85 minutes using a personal computer of 2.66 GHz. However, for real complex geometries as shown in figures 16-18, a lot of time is employed to check whether a point is inside (or not) of the 3D boundary. Then, it is necessary to implement methods for improving the efficiency of the algorithm (see Goodman and Rourke, 1997). This is currently being done.
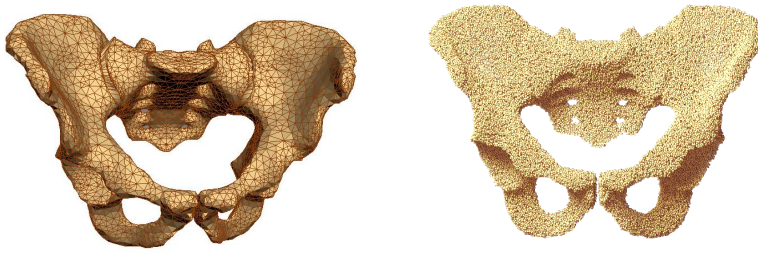
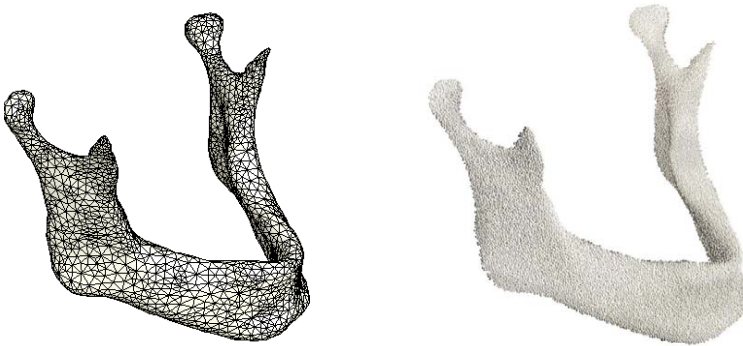Figure 17: Human hip: a) boundary element mesh b) 349748 particles model

Figure 18: Human mandible: a) boundary element mesh b) 73605 particles model

4   Discussion and Conclusions

In this research some particle-packaging methods for simulations and analysis with the Discret Element Method of human bones have been developed and discussed. The methods allow the user to consider very complex geometries and orthotropy. The methods were validated by modeling the human skull, hip and mandible.

When dealing with spongy (trabecular) bone, the use of elliptical holes carried out after very compact packages of circles or spheres was extremely useful for modeling this kind of bone. On the other side, compact bone has been successfully modeled using very dense particle-packages. The denser the package obtained, the better the results obtained for compact bone. This is the first step to model and to analyze complex geometries of human bones, just before the structural simulation.

The spatial orientation of the ellipsoids is of the most concern to deal with the modeling of bone mechanical properties. Spheres are not recommended to achieve this goal.

Further research is deserved (and mandatory) to get a more precise understanding of spongy bone behavior and geometry, in order to obtain more accurate statistical distributions for the particles, since there is no a direct relationship between the dimensions of the particles and many geometric and mechanical characteristics of spongy bone.

Perhaps, one of the key aspects regarding the efficiency of this kind of algorithms is to optimize the verification if a particle is inside (or not) of the 3D boundary. This is a time consuming process and further mathematical and computational effort is being done to reduce the CPU time in this step.

References

Cowin S.C., Hegedus D.H. (1976), Bone remodeling I: a theory of adaptive elasticity, *J. Elasticity,* **6**:313–326

Feng Y.T., Han K., Owen D.R.J. (2002), An advancing front packing of Polygons, Ellipses and Spheres, *In Discrete Element Methods*, Cook BK, Jensen RP (eds). ASCE: New York; pp. 104-106

Feng Y.T., Han K., Owen D.R.J. (2003), Filling domains with disks: an advancing front approach, *Int. J. Numer. Meth. Engng,* **56**:699-713

Ferrez J.A. (2001), *Dynamic triangulations for efficient 3d simulation of granular materials*, Thèse Doctoral N°. 2432, Département de Mathématiques, Lausanne, École Polytechnique Fédérale de Lausanne, Switzerland.

Ferrez J.A., Liebling T.H. (2002), Dynamic triangulations for efficient detection of collisions between spheres with application in granular media simulations, *Philosophical Magazine,* **B 82 (8):**905–929

Goldstein S.A., Matthews L.S., Kuhn J.L., Hollister S.J. (1991), Trabecular bone remodeling: an experimental model, *J. Biomech.* **24** (Suppl 1):135–150

González Y., Cerrolaza M., González C. (2009), Poroelastic analysis of bone tissue differentiation by using the boundary element method, *Eng. Anal. Bound. Elem.,* **33:**731-740

Goodman J. E., O'Rourke J. (1997) (editors), Handbook of Discrete and Computational Geometry, *CRC Press LLC*, section 30, Florida, USA

Han K., Feng Y.T., Owen D.R.J. (2005), Sphere packing with a geometric based compression algorithm, *Powder Technology* **155**: 33-41

Jerier J.F., Richefeu V., Imbault D., Donzé F.V. (2010), Packing spherical discrete elements for large scale simulations, *Comp. Meth. App. Mech. & Eng.,* **199**:1668-1676

Löhner R., Oñate E. (2004), A general advancing front technique for filling space with arbitrary objects, *International Journal for Numerical Methods in Engineering*; **61**:1977-1991

Martínez G., Cerrolaza M. (2006), A bone adaptation integrated approach using BEM, *Eng. Anal. Bound. Elem.,* **30:**107-115

Martínez G, García J., Doblaré M., Cerrolaza M. (2006), External bone remodeling through boundary elements and damage mechanics, *J. Math. Comp. Sim.,* **73:**183-199

Nandakumar K., Shu Y., Chuang K.T. (1999), Predicting geometrical properties of random packed beds from computer simulation, *AIChE Journal*, **45**(11):2286-2297

Pérez I., Roselló R., Pérez Y., Díaz-Guzmán H., Recarey C. (2009), A generic particles-packaging procedure for the discrete element method (in Spanish), *Rev. Int. Mét. Num. Calc. Dis. Ing.*, **25**(2):95-110

Perkins E., Williams J.R. (2001), A fast contact detection algorithm insensitive to object sizes, *Engineering Computations*, **18**(1/2):48-61

Siiriä S., Yliruusi J. (2007), Particle packing simulations based on Newtonian mechanics, *Powder Tech,* **174:**82-92

Sutou A., Dai Y. (2002), Global optimization approach to unequal sphere packing problems in 3D, *Journal of Optimization Theory and Applications.* **114**(3):671-694

Wang Ch.Y., Liang V-Ch. (1997), A packing generation scheme for the granular assemblies of planar elliptical particles, *Int. J. Numer. Anal. Meth. Geomech.*, **21**:347-358

Wang, Ch-Y., Wang L., Sheng J. (1999), A packing generation scheme for the granular assemblies with 3d ellipsoidal particles, *Int. J. Numer. Anal. Meth. Geomech.*, **23**:815-828