3D MULTISCALE VECTORIAL SIMULATIONS OF RANDOM MODELS

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ABSTRACT

We present here a method using level sets as primary grains to generate 3D simulations of random models in the continuous space. Primary grains of any shape can be used as long as we are able to represent them by an implicit function. Simulations are generated using Boolean combinations of the primary implicit functions. This approach allows us to build complex combinations of simulations that we could not obtain with a pixel based method. Furthermore, vectorial simulations do not require a large amount of computer resources, which allows us to obtain fast generations of microstructures with very large sizes and numbers of primary grains.

KEYWORDS: Random models, vectorial simulation, implicit functions.

INTRODUCTION

The heterogeneity of materials can be handled through a probabilistic approach to generate models and simulations of the microstructures, before estimating their physical behavior. An efficient way to model random media is based on the theory of random sets [1, 2], giving a strong theoretical framework for modeling heterogeneous microstructures by means of a probabilistic approach. Such simulations are generally performed in the discrete space on a grid of points (2D or 3D images) [3, 4], using combinations of pixel based primary grains.

The aim of this paper is to introduce tools allowing to generate 3D random models in the continuous space using level-sets. Primary grains are defined by implicit functions. Boolean combinations of base implicit functions are used to build 3D random models. The models generated are also implicit functions and then they can be represented as well with level-sets and can be exported directly as mesh or as 3D images. Generated models can also be used for embedded models or be themselves implanted as primary grains to produce more complex structures. Examples of multiscales simulations obtained with this method will be presented in this paper.

IMPLICIT FUNCTIONS

Implicit functions are real valued functions defined in 3D space by $\varphi(x,y,z) = c$. An implicit function representation [5] defines a surface as a level set of a function φ, most commonly the set of points for which $\varphi(\vec{x}) = 0$.

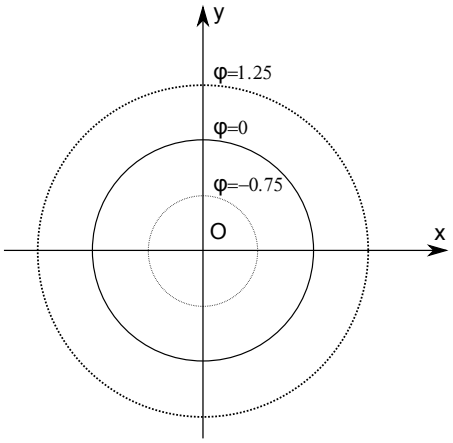


Figure 1. *Representation of the 2D implicit function* $\varphi(x,y) = x^2 + y^2 - 1$ *with three level sets:* $\varphi = -0.75$, $\varphi = 0$ *and* $\varphi = 1.25$.

Two primitive operations are required: the ability to evaluate the function, and the function gradient at a given point. The implicit function divides space into three regions:

- on the surface: $\varphi(x,y,z) = c$,
- outside of the surface: $\varphi(x,y,z) > c$,
- and inside the surface: $\varphi(x,y,z) < c$.

When c is zero, positive values are outside, negative values are inside, and zero is on the surface (as illustrated with a sample function in figure 1). Note also that the function gradient points from inside to outside.

BOOLEAN OPERATIONS ON IMPLICIT FUNCTIONS

If φ_A and φ_B are two different implicit functions, then the implicit function $\varphi_{A \cup B}$ representing the union

of the interior region of φ_A and φ_B is defined by:

$$\varphi_{A\cup B}(\vec{x}) = min(\varphi_A(\vec{x}), \varphi_B(\vec{x}))$$

Similarly, the implicit function $\varphi_{A\cap B}$ representing the intersection of the interior regions of φ_A and φ_B is defined by:

$$\varphi_{A\cap B}(\vec{x}) = max(\varphi_A(\vec{x}), \varphi_B(\vec{x}))$$

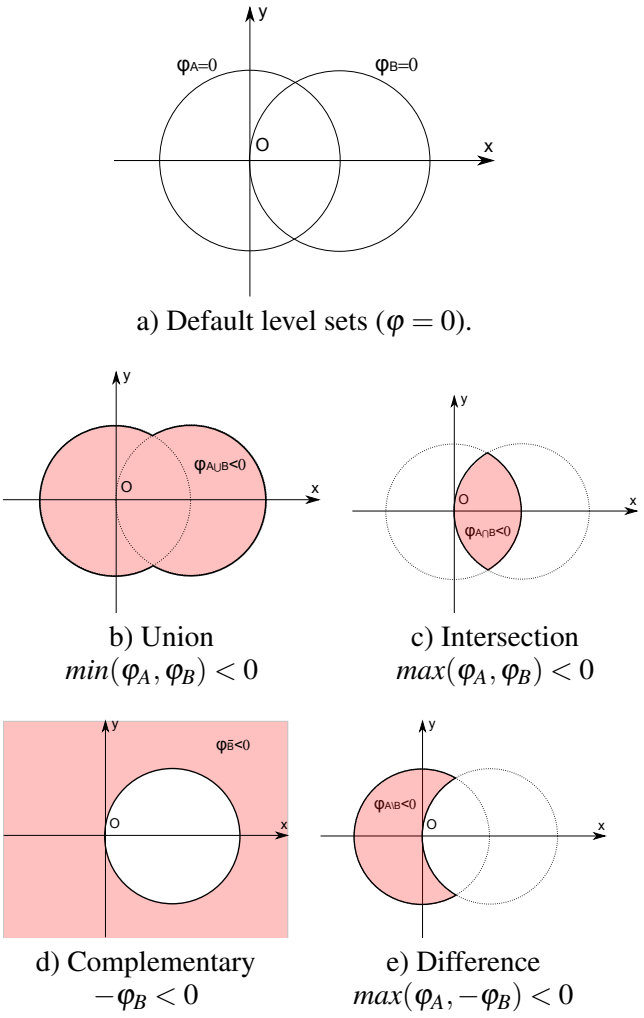
The complementary $\varphi_{\bar{A}}$ of an implicit function φ_A corresponds to its opposite function:

$$\varphi_{\bar{A}}(\vec{x}) = -\varphi_A(\vec{x})$$

which allows us to define the difference function $\varphi_{A\setminus B}$:

$$\varphi_{A\setminus B}(\vec{x}) = \varphi_{A\cap\bar{B}}(\vec{x}) = max(\varphi_A(\vec{x}), -\varphi_B(\vec{x}))$$

The figure 2 represents examples of Boolean operations on two implicit functions.



a) Default level sets ($\varphi = 0$).

b) Union $min(\varphi_A, \varphi_B) < 0$

c) Intersection $max(\varphi_A, \varphi_B) < 0$

d) Complementary $-\varphi_B < 0$

e) Difference $max(\varphi_A, -\varphi_B) < 0$

Figure 2. *Boolean operations with two implicit functions:* $\varphi_A(x,y) = x^2 + y^2 - 1$, *and* $\varphi_B(x,y) = (x-1)^2 + y^2 - 1$

RANDOM SETS MODELS

POINT PROCESSES

Point processes are the first step in the construction of more general models, that are called grain models. Considering a compact set $K = [0, X_{max}] \times [0, Y_{max}] \times [0, Z_{max}] \subseteq \mathbb{R}^3$ and a probability space $(\Omega, A, \mathbb{P})$, a point process X is defined as a mapping from the probability space to configurations of points of K:

$$\forall \omega \in \Omega, X(\omega) = \{x_1, \ldots, x_n, \ldots\}, x_i \in K$$

Poisson point process

One of the most prevalent and simple stochastic model for the creation of spatial point patterns is the Poisson point process. This point process allows to simulate a complete spatial randomness, which is usually inaccessible in practice. The nonhomogeneous Poisson point process in $\mathbb{R}^n$ with a regionalized intensity $\theta(x)$ ($x \in \mathbb{R}^n$, $\theta \geq 0$) is such that the numbers $N(K_i)$ are independant random variables for any family of disjoint compact sets K_i. $N(K)$ is a Poisson random variable with parameter $\theta(K)$:

$$\theta(K) = \int_K \theta(dx) \tag{1}$$

$$P_n(K) = P\{N(K) = n\} = \frac{\theta(K)^n}{n!} exp(-\theta(K)) \tag{2}$$

Hardcore point process

For the Matern hard core point process, the points are located in a more regular way than in the case of the Poisson point process. A possible principle for hard core processes is done by thinning the points of a Poisson point process [6]. This can be accomplished by considering a specified hard core distance. This means that only points which have a certain minimum distance to their nearest neighbour are retained. This may be interpreted to imply certain repulsion effects between the points. Two parameters describe a Matern hard core point process: the intensity θ of the underlying Poisson point process and the hard core distance D. Then, the intensity, θ_{MH} of the Matern hard core point process is given by [6]:

$$\theta_{MH} = \frac{1 - e^{-\theta D^2 \pi}}{D^2 \pi} \tag{3}$$

BOOLEAN MODEL

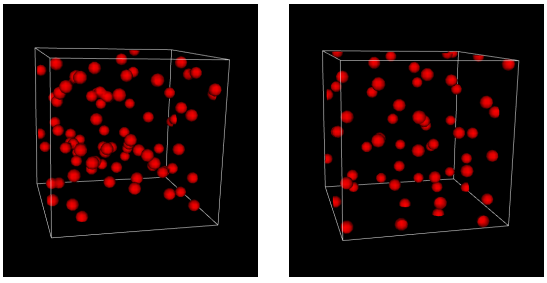
The Boolean model [1, 2, 6] is obtained by implantation of random compact primary grains A' (with possible overlaps) on Poisson points x_k with the intensity θ, giving the random set $A = \cup_{x_k} A'_{x_k}$. The figure 3 show realizations of simple Boolean models using spheres as primary grains. For each Poisson point $P_i(x_i, y_i, z_i)$ generated, we define an implicit function

$$\varphi_i(x,y,z) = (x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2 - R_i$$

(where R_i is the radius of the sphere implanted at point P_i).

The Boolean model will correspond to the union of the spheres, that is to say, to the function φ_{bool} defined by:

$$\varphi_{bool}(x,y,z) = min(\varphi_i(x,y,z))$$



a b

Figure 3. *Boolean model of spherical primary grains generated in a unit cube: a) using simple Poisson point process ($\theta = 0.08$). b) using hardcore Poisson point process ($\theta = 0.08$, $D = 0.25$). The radius is the same for all implanted spheres: $R_i = 0.04$. The surfaces represented correspond to the default level set of the function φ_{bool}: $\varphi_{bool}(x,y,z) = 0$.*

MULTISCALE BOOLEAN MODEL

Multiscale Boolean models are binary version of Cox Boolean models, where the homogeneous Poisson point process is replaced by a Cox point process (Poisson process with a non-uniform intensity $\theta(x)$) [7]. They are generated using embedded one-scale Boolean models: a first microstructure made of a Boolean set of primary grains is generated (with a point density θ_1). The union of those first primary grains is used as a binary mask for the point process of the second scale model: the second set of Poisson points are genrated with the following intensity:

- $\theta(x) = \theta_2$ inside the first-scale grains,
- $\theta(x) = 0$ outside the first-scale grains.

Every Boolean combination of implicit functions is itself an implicit function. Thus, a function φ_{bool} resulting from a Boolean combination of implicit functions φ_i preserves the property of space division: φ_{bool} is positive at every point outside of its surface, null on the surface and negative at every point interior to its surface.

In order to simulate a multiscale Boolean model, a first one-scale Boolean model is generated. The resulting implicit function φ_{bool_1} is used as a mask for a second point process: here again, we generate randomly new Poisson points in the whole space, but only points that are within the surface of φ_{bool_1} are kept. In other words, a point x_k generated during the second Poisson point process is kept only if $\varphi_{bool_1}(x_k) < 0$.

Such construction is illustrated in figure 4 with two embedded Boolean models with spherical primary grains. The same method can be employed with any number of scales and any base models: the figure 5 shows an example of a two-scale Boolean model obtained with a combination of a Poisson line process and a Boolean model of spheres.

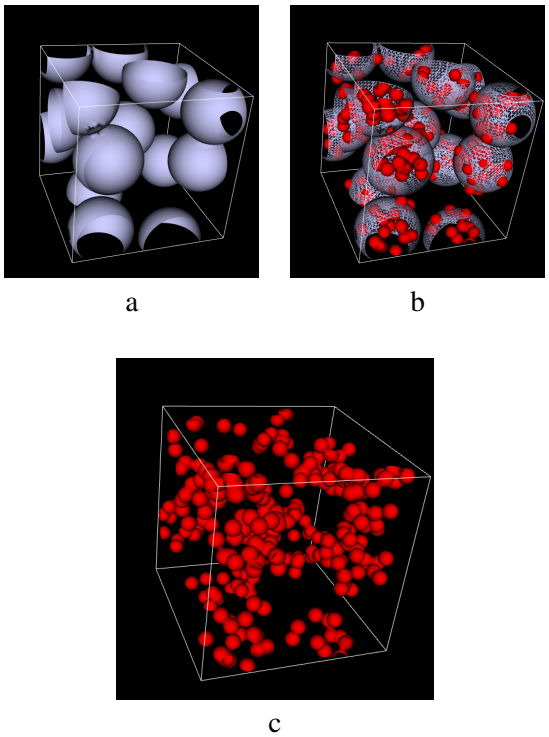


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Figure 4. *Two-scale Boolean model of spheres (generated in a unit cube). a) First scale (hardcore) Boolean model: density of the Poisson point process: $\theta_1 = 0.01$, hard-core distance: $d_1 = 0.4$, radius of spheres (constant): $r_1 = 0.2$. b) Generation of the second scale Boolean model (red, plain) within the first one (blue, wireframe): $\theta_2 = 0.9$, $d_2 = 0$, $r_2 = 0.04$. c) Resulting two-scale Boolean model.*

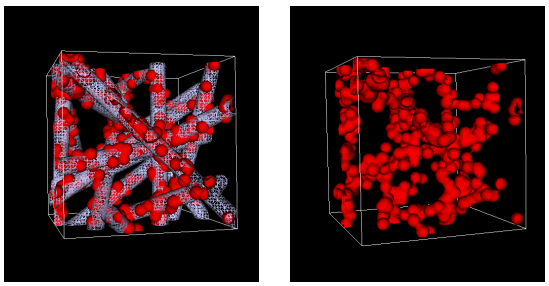

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Figure 5. *Two-scale Boolean model obtained with a Poisson lines process (blue, wirelines) embedded with a Boolean model with spherical primary grains (red, plain). a) Combined view. b) Resulting union of spheres.*

ADVANTAGES OF THE METHOD

This method of simulation is quite flexible, and allows to generate realistic random media with a low computational effort and memory storage. Quite large simulations can be obtained, in order to reproduce random media involving a superimposition of scales, as well as a wide range of sizes, since there is no impact of the digitization in the simulations. Furthermore, boundaries of generated microstructures are meshed, which makes the simulations a suitable input in a finite element code for the numerical prediction of the effective properties of complex microstructures [8]. Moreover, when generated models are used in physical simulations, it is often necessary to produce periodic models, and if the generation of periodic models is also possible in the discrete case, only the level set based approach can ensure to produce periodic meshes. The simulation approach is not restricted to binary random sets, and was extended to tesselations, multi-component media, such as the dead leaves model [4] (as illustrated by figure 6), ...

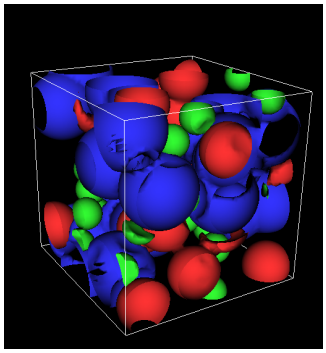

Figure 6. *Three phases dead-leaves model of spheres*

CONCLUSIONS

We presented a method allowing to generate 3D simulations of random models in the continuous space using level sets. Primary grains are described by implicit functions, which are combinated by Boolean operations to produce random 3D models. As both primary grains and the generated models are implicit functions, possibilities of combinations offered by this method are infinite and allows us to produce models with a high complexity. The vectorial approach is quite flexible and does not require a large amount of computer ressources.

The results presented here were obtained using the VTKSIM library. This library, developped at the Centre de Morphologie Mathématique, is built as an on layer of the VTK (Visualization ToolKit) library [9]. A demo version presenting some of its capabilities is available online: http://cmm.ensmp.fr/~faessel/vtkSim/demo/

REFERENCES

[1]Georges Matheron, *Elements pour une theorie des milieux poreux*, Masson, Paris, 1967.

[2]Georges Matheron, *Random sets and integral geometry*, J. Wiley, New York, 1975.

[3]T. Nion, D. Jeulin, and G. Fricout, "SIMEA: an advanced framework for random media simulation," in *Proceedings of the 8th International Symposium on Mathematical Morphology*, Rio de Janeiro, Brazil, Oct. 2007, vol. 2, pp. 53–54.

[4]Dominique Jeulin, "Random texture models for material structures," *Statistics and Computing*, vol. 10, no. 2, pp. 121–132, Apr. 2000.

[5]Stanley J Osher and Ronald P Fedkiw, *Level Set Methods and Dynamic Implicit Surfaces*, Springer, Oct. 2002, Published: Hardcover.

[6]Dietrich Stoyan, *Stochastic Geometry and its Applications.*, John Wiley & Sons, Chichester, 2nd edition, 1995.

[7]D. Jeulin, "Modeling heterogeneous materials by random structures," in *European Workshop on Application of Statistics and Probabilities in Wood Mechanics*, Bordeaux, Mar. 1996, Paris School of Mines Publication, Invited lecture.

[8]A. Jean, D. Jeulin, S. Forest, S. Cantournet, and F. N'Guyen, "A multiscale microstructure model of carbon black distribution in rubber," *Journal of Microscopy*, vol. 241, no. 3, pp. 243–260, 2011.

[9]Will Schroeder, K. W. Martin, and W. Lorensen, *The visualization toolkit : an object-oriented approach to 3D graphics*, Kitware, 3rd edition, 2002.