Geometrical Stochastic Modeling and Characterization of 2-D Crystal Population

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Introduction

The presented work is motivated by a pharmaceutical issue. Indeed, the production of drugs involves a crystallization process in solution depending on several parameters and their quality is closely linked to its geometrical characteristics (size, shape, quantity ...). Therefore, it is necessary to control the distribution of the "crystal geometry" during the process. To meet this goal, an in-situ optical acquisition system provides images of the crystal population crystals' population, giving access to the projected particles during the process (see Figure 1). These images highlight the overlapping of the crystals (caused by the 2-D projection) and it is consequently difficult to individualize the particles for further characterization. Therefore, after a binarization process [1] (see Figure 1), the objective of this work is to investigate stochastic geometrical models so as to represent these binary images and to get the geometrical characteristics of the crystals.

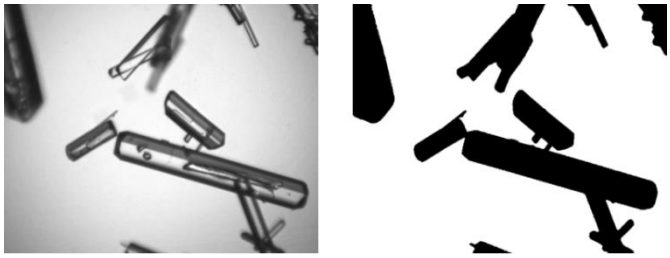

Figure 1. Acquisition of an image of a crystals' population and its segmentation.

Modeling and objectives

Several materials can be modeled by random sets. In fact, the heterogeneity of the materials can be apprehended by a probabilistic approach [2],[3]. Especially granular or fibrous media [4],[5] can be represented by unions of overlapping particles (the grains) centered on random positions (the germs), thus giving rise to the germ-grain model.

$$\Xi = \bigcup_{x_i \in \Phi} x_i + \Xi_i \qquad (1)$$

Where Φ is a point process which generates the germs x_i, and where the grains Ξ_i are convex random sets independent and identically distributed.

Notice that this definition assumes the independence between the particles Ξ_i and their positions x_i there is a more general definition authorizing the correlation between germs and grains [6].The proposed approach consists in representing the population of crystals by such a germ-grain model (Figure 2); that is to say that the point process Φ represent the spatial distribution of the particles centers and the convex random sets Ξ_i the particles themselves. The goal is to adjust the model to the real data by matching measurements computed both on real and simulated images. The real data are here obtained by an imaging acquisition system, meaning that we have only realizations of $\Xi \cap W$ where W is a bounded window, and we want to estimate the characteristics of Φ and Ξ_0.

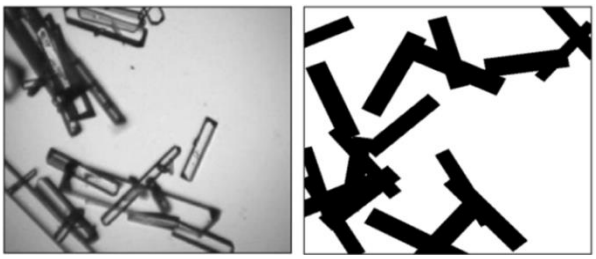

Figure 2. Acquisition of an image of a crystals' population, and realization of a geometric stochastic model representing it.

To meet this objective, we focus on two points: firstly, we estimate the characteristics of Ξ from a realization of $\Xi \cap W$ [7], secondly we establish relationships between the characteristics of Ξ and the local characteristics of the model (Φ and Ξ_0). We also introduce an additional assumption: we assume the process Φ comes from a known type (Poisson process, Cox process ...). We will use the homogeneous Boolean model, a germ-grain model in which Φ is a homogeneous Poisson point process. This model is widely used because we have an analytical formula for the Choquet capacity.

$$T_{\Xi}(X) = 1 - \exp(-\lambda\, \mathbb{E}[A(\Xi_0 \oplus K)]) \tag{2}$$

Several methods have been presented in the literature so as to connect the global characteristics of the Boolean model to the characteristics of the primary grain. In the plane and the space, the Miles's formulae [8] or the minimum contrast method [9] provide theoretical relationships to estimate the average values of the Minkowski functionals of the primary grain from global characteristics. Generally, the primary grain is assumed to have a known and deterministic shape, that is to say, the realizations of the primary grain are homothetic. So as to estimate the variations of the scaling factor from the expectation of the Minkowski functionals. For example, for a disc in the plane, the moments of the first and second orders of the radius of the primary grain are respectively proportional to its average perimeter and its average area. However, if we consider that the shape of the grain can vary, several issues remain unresolved: firstly the Minkowski functionals of a random convex set are not enough to characterize its shape and also their average will not provide sufficient information to characterize its variations. For instance, for a Boolean model whose grains has a shape that depends on several parameters (rectangle, ellipse ...); the estimation of geometric variations of the grain is not straightforward.
The proposed work provides estimators of the geometrical variations of the primary grain of the Boolean model without any assumption concerning its shape.

Method and results

It's well known that the second order moment of the area of the primary grain can be expressed as the integral of the mean geometric covariogram [10]:

$$\mathbb{E}[A(\Xi_0)^2] = \int_{\mathbb{R}^2} \gamma_{\Xi_0}(u)du \tag{3}$$

Where $\gamma_{\Xi_0}(u) = \mathbb{E}[A(\Xi_0 \cap \Xi_0 + u)]$ is the mean geometric covariogram of Ξ_0. Thus, under the hypothesis $\mathbb{E}[A(\Xi_0)] < \infty$ it is possible to obtain an estimator for $\mathbb{E}[A(\Xi_0)^2]$ from an estimator of $\gamma_{\Xi_0}(u)$. In the special case of the Boolean model the mean geometric covariogram can be obtain by the covariance $C_{\Xi}(u)$, also called 2-points probability function by the following relation associate to Miles's estimator of intensity.

$$\gamma_{\Xi_0}(u) = \frac{1}{\lambda} \ln\left(1 + \frac{C_{\Xi}(u) - p_{\Xi}^2}{(1 - p_{\Xi})^2}\right) \tag{4}$$

Where $p_\Xi = C_\Xi(0)$ is the fraction area of Ξ. Let's notice that the Boolean is stable by convex dilatation; that is to say, for each compact convex set K the random set $\Xi \oplus K$ is also a Boolean model of same intensity λ and of primary grain $\Xi_0 \oplus K$. Consequently for any compact convex set K the quantities $\lambda, \mathbb{E}[A(\Xi_0 \oplus K)]$ and $\mathbb{E}[A(\Xi_0 \oplus K)^2]$ are estimable. Especially, considering a family of homothetic convex compact sets $(rK)_{r>0}$ the second order moment of the area of dilated grain $\mathbb{E}[A(\Xi_0 \oplus rK)^2]$ is a polynomial function in r, and can be expressed by Steiner's formula as follows:

$$\mathbb{E}[A(\Xi_0 \oplus rK)^2] = \mathbb{E}[A(\Xi_0)^2] + 4r\mathbb{E}\left[A(\Xi_0)W_{0,K}\right] + r^2\left(4\mathbb{E}\left[W_{0,K}^2\right] + 2A(K)\mathbb{E}[A(\Xi_0)]\right) + 4r^3A(K)\mathbb{E}\left[W_{0,K}\right] + r^4A(K)^2 \quad (5)$$

where $W_{0,K}$ is the mixed area between Ξ_0 and K [11],[12]. The quantities $\mathbb{E}[A(\Xi_0)]$ and $\mathbb{E}\left[W_{0,K}\right]$ can be estimated by the minimum contrast method [13] or by the Miles's formulae [6]. Consequently the quantities $\mathbb{E}[A(\Xi_0)^2], \mathbb{E}\left[A(\Xi_0)W_{0,K}\right]$ and $\mathbb{E}[W_{0,K}^2]$ can be estimated by a polynomial approximation of $\mathbb{E}[A(\Xi_0 \oplus rK)^2]$. In practice the choice of the values of r play an important role, and a precaution for the edge effect must be taken into account; if $\Xi(\omega) \cap W$ is a realization of Ξ in a bounded windows W, the dilated model $\Xi \oplus rK$ is only known on the eroded windows $W_r = W \ominus rK$ and its realization in the windows W_r is $(\Xi(\omega) \cap W) \oplus rK) \cap W_r$.

The choice of the convex compact set K provides different characteristics of the primary grain; for a ball, the mixed area $W_{0,K}$ is proportional to the perimeter $U(\Xi_0)$, and for a segment oriented by $\theta \in [0,2\pi]$, it is proportional to the Feret's diameter of Ξ_0 in the direction θ.

This method can be generalized to obtain n^{th}order moments of $(A(\Xi_0), W_{0,K})$, using n-points probability functions (article in preparation).We have evaluated the performance of the proposed method for a disk and a segment by simulating several realizations of a test model in a squared window 500×500. The test model is isotropic model with a point process intensity $\lambda = 100/500 \times 500$ and with rectangular grains whose side lengths are independent and follow the Gaussian distributions $N(40,10)$ and $N(30,10)$. The results are presented in Figure 3, where the relative errors on the geometrical variations of the grains are shown as a function of the number of realizations.

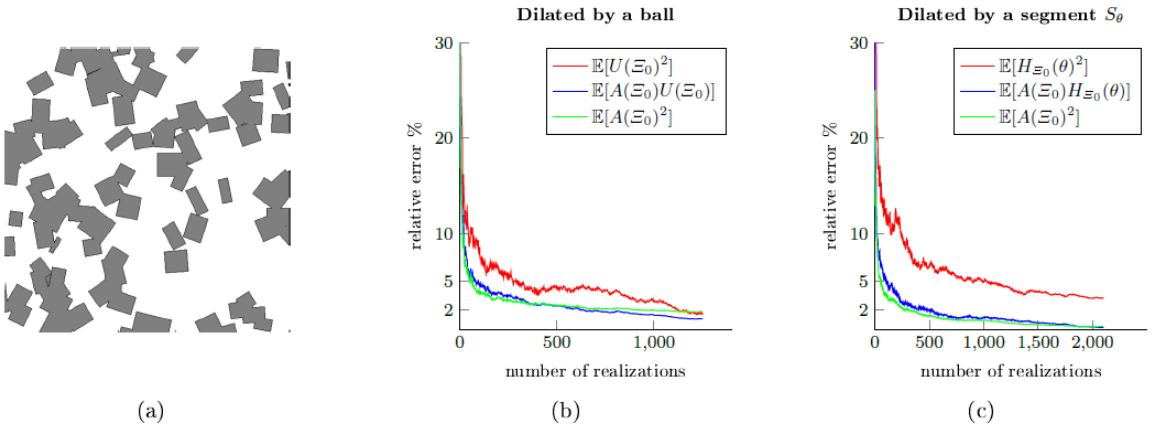

Figure 3. A realization of the test model (a) and the relatives errors of the second order moments of (area, perimeter) on (b) and of (area, Feret's diameter) on (c).

Conclusions and prospects

A method has been presented so as to geometrically model and characterize a population of crystals. It provides estimators of the variations of the primary grain's morphological characteristics. Especially, using dilatation by a disk or a segment, the proposed method can be used to better characterize the geometry of a

primary grain whose shape depends on two parameters (rectangle, ellipse...). We emphasize that our method can be used for any germ-grain model in which we can estimate the mean covariogram. In the future we are looking for more complex germ-grain models than the Boolean model. We are also interested in the influence of the model parameters and the observation window on the accuracy of the estimations. The prospect of describing a convex random set by the characteristics of the random process associated to its Feret's diameters seems to be also promising.

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