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A novel numerical scheme for random parameterized convex aggregate models with a high-volume fraction of aggregates in concrete-like granular materials

Huaifa Ma [a], Laizhong Song [b], Wenxiang Xu [a,c,*]

[a] State Key Laboratory of Simulation and Regulation of Water Cycle in River Basin, China Institute of Water Resources and Hydropower Research, Beijing 100048, China
[b] College of Science, China Three Gorges University, Yichang 443002, China
[c] College of Mechanics and Materials, Hohai University, Nanjing 211100, China

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ABSTRACT

Concrete at a mesoscopic scale is normally regarded as a three-phase composite consisting of cement paste, aggregates and their surrounding interfacial transition zones (ITZs). Establishing mesostructure model close to realistic concrete is very crucial to precisely evaluate its mechanical properties. The preponderance of previous investigations has focused on aggregates as circles, ellipses or polygons constructed by the assembly of sides-sides with a low packing density, and little is known about precise mathematical characterizations for polygonal aggregates with a high packing density more than 60% and their surrounding ITZs. In this work, a novel numerical framework that adopts the deformation of a rhombus to mathematically provide a parametric equation of convex polygon characterizing the geometrical morphology of aggregates, is proposed to generate random polygonal aggregate models (RPAMs) with a high packing density. In this framework, a fast-random packing algorithm (FRPA) is developed to generate a high packing density of aggregates of 70%. Based on the parametric equation of polygonal aggregates, the geometrical topology of ITZs is mathematically realized with a convenient manner, rather than those cumbersome approximate operations reported in the literature. Moreover, the present numerical framework can be extended to the three-dimensional case.

1. Introduction

Aggregates are always used in concrete, mortar, ceramic and some other granular materials. Aggregates play an important role in improving mechanical properties of concrete [1–3]. At a mesoscopic scale, plain concrete is usually regarded as a three-phase composite structure consisting of cement paste, aggregates and interfaces around individual aggregates [4–7]. Practically, aggregates possessing diverse geometrical shapes and dimensions are randomly distributed in cement paste that forms a mesostructure of concrete [8–11]. The establishment of mesostructure model close to realistic concrete is very crucial to precisely estimate the structural characteristics and mechanical properties of concrete.

As early as 1985, Wittmann and his collaborators [12] developed some aggregate models including circles, polygons, and some other irregular shapes. Afterwards, Wang et al. [13] simulated two-dimensional (2D) complex polygons representing aggregates. Wang et al. [14,15] described a "generate-and-place" procedure to simulate 2D and 3D (three-dimensional) composites with random distribution of circular/spherical/, elliptical/ellipsoidal and polygonal/polyhedral grains. In addition, Xu et al. [16,17] developed two robust overlapping detection criterions to construct random sequential packing models of ellipsoids and regular convex polyhedra, respectively. Such random sequential packing models were further applied to numerically evaluate the microstructures and physico-mechanical properties of concrete [6,11,18–23]. These progresses have been summarized in the recent review article [24]. Moreover, the authors [25] recently proposed a 2D random non-convex aggregate model to evaluate the fraction of interfacial transition zones (ITZs) around aggregates. However, these methods have the same disadvantages that the packing density and shape of the simulated aggregates are far from that of the real aggregates. It is well known that the better approximations on the shape and packing density of aggregates can reliably generate the statistical properties of concrete. Considering common crushed stone aggregates, researchers have introduced polygonal and polyhedral

* Corresponding author at: College of Mechanics and Materials, Hohai University, Nanjing 211100, China.

E-mail addresses: mahf@iwhr.com (H. Ma), slz@ctgu.edu.cn (L. Song), xwxfat@gmail.com (W. Xu).

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aggregate models [7,9,13–15,17,21], which closely resemble the actual shape of aggregates. These polygonal or polyhedral models are mainly constructed by the assembly of sides-sides or sides-planes. However, the precise mathematical characterization for the polygonal or polyhedral aggregate models is rarely involved in previous contributions.

In this article, the authors attempt to develop parametric equations to quantitatively control geometric models of convex polygonal aggregates through the deformation of a rhombus-based convex polygon, instead of the traditional assembly of sides-sides. The advantages of such the operation cannot only realistically describe the shape of crushed aggregates, but also precisely characterize the morphology of ITZ around each crushed aggregate. Additionally, taking advantages of such the parametric representation, the position relationship between aggregates can be easily identified by calculating the distance between an arbitrary spatial point and a generated aggregate. On the other hand, the authors propose some optimized packing strategies to improve the packing density of aggregates. The numerical tests show that the proposed methods can generate random polygonal aggregate models (RPAMs) with a high packing density which is very close to the practical structure of concrete. Moreover, RPAMs can be further extended to 3D case.

The rest of this article is organized as follows. Section 2 describes the parameterized geometrical morphology of a polygonal aggregate. The relative position between one point and a polygon and the overlap detection of adjacent polygons are elaborated in Section 3. Section 4 illustrates random polygonal aggregate models with a high packing density in detail. Section 5 presents a mesostructure models of concrete by using the proposed algorithms. Section 6 extends the present 2D RPAMs to the 3D case. Finally, this article is completed with some concluding remarks in Section 7.

2. Algorithmic foundation

To begin, the authors describe the parametric equation of a generalized ellipse:

$$\frac{|\cos\alpha(x-x_0)+\sin\alpha(y-y_0)|^{s_1}}{|r_1|^{s_1}} + \frac{|-\sin\alpha(x-x_0)+\cos\alpha(y-y_0)|^{s_2}}{|r_2|^{s_2}} = 1 \tag{1}$$

where s_1, $s_2 > 0$, r_1, $r_2 \neq 0$, $O(x_0, y_0)$ is the centre of generalized ellipse, $\alpha \in [0, \pi]$ is the included angle between the principal axis of ellipse and x-axis, as shown in Fig. 1. When $s_1 = s_2 = 2$, the generalized ellipse is an ordinary ellipse. If $s_1 = s_2 = 1$, it is a rhombus and its diameter is defined as

$$R = 2\max\{|r_1|, |r_2|\} \tag{2}$$

Assuming $r_1 > r_2 > 0$, the parametric equation of rhombus is described by

$$P(\theta) = \begin{pmatrix} x(\theta) \\ y(\theta) \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} \frac{r_1\cos\theta}{|\cos\theta|+|\sin\theta|} \\ \frac{r_2\sin\theta}{|\cos\theta|+|\sin\theta|} \end{pmatrix} + \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, \quad \theta \in [0, 2\pi] \tag{3}$$

the function is considered by

$$g(x,y) = \frac{|\cos\alpha(x-x_0)+\sin\alpha(y-y_0)|}{|r_1|} + \frac{|-\sin\alpha(x-x_0)+\cos\alpha(y-y_0)|}{|r_2|} - 1 \tag{4}$$

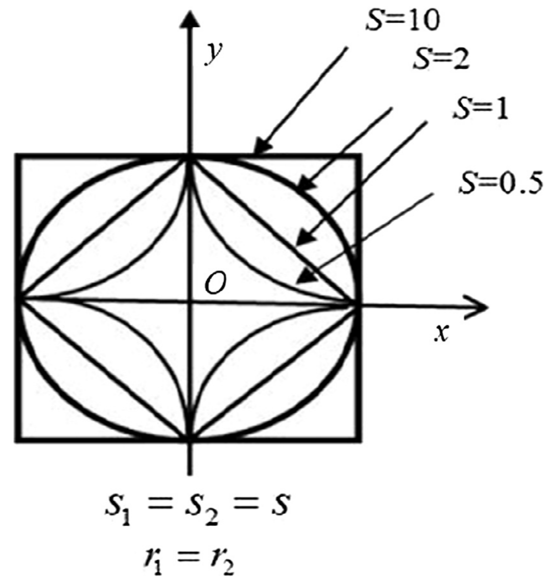

Fig. 1. Two-dimensional generalized ellipse.

Then, for the point $P(x, y)$ on the plane, the following proposition is dictated: If $g(x, y) > 0$, P is outside the rhombus; if $g(x, y) = 0$, P is on the boundary of rhombus; otherwise, P is inside the rhombus.

To obtain a convex polygon by Eq. (3), the authors assume I_i: $[a_i, b_i] \subset [0, 2\pi]$, $i = 1, \ldots, n$, and set

$$\lambda_i(\theta) = \frac{x(a_i)y(b_i) - y(a_i)x(b_i)}{x(\theta)[y(b_i) - y(a_i)] - y(\theta)[x(b_i) - x(a_i)]} \tag{5}$$

As shown in Fig. 2, the original polygon keeps constant if the difference between the vector $P(b_i)$ and the vector $P(a_i)$ on the sides of rhombus; otherwise the rhombus will be changed if the difference is not on the sides. Also, such the deformation can be continuously superposed, resulting in a parametric equation of arbitrary convex polygon. The deformed curve P_d is given by

$$P_d(\theta) = \sum_{i=1}^{n}\{B_i(\theta)\lambda_i(\theta)P(\theta) + [1 - B_i(\theta)]P(\theta)\}, \quad \theta \in [0, 2\pi] \tag{6}$$

where

$$B_i(\theta) = \begin{cases} 1 & \theta \in I_i \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

where $B_i(\theta)$ is the translation on the I_i. as shown in Fig. 2.

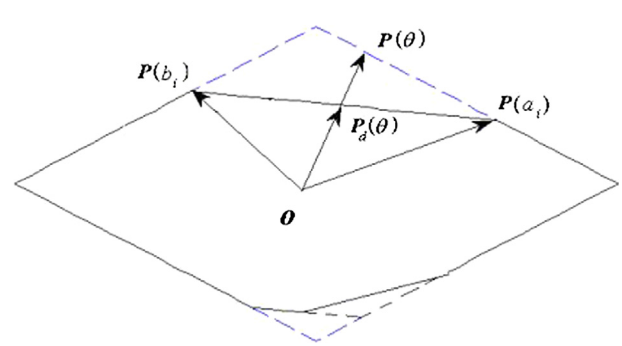

Fig. 2. Polygon obtained by the deformation and superposition of rhombus.

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