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Research Paper

Packing of discrete and irregular particles

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ABSTRACT

A new conditional modeling along with a level-set method that can produce high quality and large packs of irregular particles is proposed. First, an initial pack of particles is generated statistically using the particles provided through an X-ray image. Then, the mismatch locations, wherein an error map identifies the particles manifest unrealistic shapes, are detected. Next, a level-set algorithm is applied to refine the defected particles using the statistical distributions extracted from the actual particles. The generated packs are statistically and physically (i.e. flow modeling) compared with the original particles and they all represent an excellent agreement.

1. Introduction

Packing of particles is a long-standing problem in various theoretical and experimental studies. One can observe such packings in every places as it has been linked to a wide range of applications such as ceramic materials [1], glasses [2], granular media [3–5], liquids [6,7], living cells [8], solids [9], suspensions [10,11], pharmaceutical industry [12], soil science [13] and so forth. The packing of uniform spheres has been studied widely in both states of random loose- and -dense packing. In the recent years, however, due to a momentous increase in computation power, modeling of more complex and, at the same time, realistic particles have become prevalent [14–19].

Boolean-based modeling is one of the popular methods that has been used to generate different particles' packs. In these techniques, the statistical properties summarizing the spatial morphology are provided based on which individual particles are generated and packed. Due to using a set of well-defined objects, the computational time of such methods is very low, and, because of the same reason, such modeling is limited to some distinct shapes. For example, circles/spheres [20–25] or cylinders [26] are two of such common particles. More complex shapes such as ellipsoids [27], polyhedrons [19,24,28–31], polyarcs [32], pentagons [33], rounded rectangles [34] have also been used. Describing the complexity and sharpness of particles, however, through these shapes cannot be achieved.

The results of particles' packing can be used in a variety of computational methods. To name a few, thermal conductivity, deformation, the interaction between particles, geomechanical analysis (e.g. stiffness, shear-induced dilatancy, shear strength, …) and flow simulation are controlled by the morphology of grains [35–38]. Such techniques cannot provide an accurate evaluation if the morphology is not represented realistically [39–42]. Furthermore, some particles may not be definable in any of the above-mentioned shapes. Thus, accurate representation of particles' complexity and shape is crucial [35,36,43,44].

The morphology of discrete particles used to be inferred from 2D scanning electron microscopic (SEM) studies [45]. Providing such images is often easy and they come with a low cost. However, extracting the necessary spatial information (i.e. 3D) out of these images may not be trustful. The recent advances in X-ray computed tomography have provided this opportunity to visualize the grains in 3D such that the spatial complexity and morphology can be extracted realistically [46–48]. For taking advantage of such images, several methods have been proposed to date that can extract the necessary information to be used within the computational techniques (e.g. discrete element method) [35,49–53]. It should be noted that using such complex particles within the computational contexts call for developing new and fast methods [34,54–57]. For example, Mollon and Zhao [58,59] have combined the theory of random fields along with a Fourier-shape-descript for generating a more realistic pack of the particle to be used within the computational frameworks. Performing all such characterizations requires the availability of 3D images and, consequently, utilizing them in the numerical simulations.

Providing several (e.g. > 10) large 3D images (e.g. $10 \times 10 \times 20\,mm^3$) of irregular particles may not be feasible in every project. Accurate and reliable evaluation in such complex media, basically, entails numerous large images to cover all the possibilities of grains' morphologies. Relying on one small and non-representative 3D image can lead to wrong predictions for catastrophic events, such as landslides, tilting, and settlement of buildings, and failure of dams, bridges and retaining walls. Thus, providing large and, at the same time, accurate models of particles is critical, as they can provide a

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deeper insight and a fundamental understanding of irregular and complex particles. Aside from the existing limitations on the size of 3D images, acquiring such large data is difficult and too expensive.

In this paper, a new attempt has been made to use the current small 3D images **I** and build several large models of discrete and irregular particles. For instance, a small image containing 670 particles is used and 50 new packs, each with 3000 particles, are generated. Unlike the previous methods, the particles are not summarized using inaccurate statistical descriptors, but they are used directly, and, if necessary, refined accordingly. To this end, a new probability-based method, within the framework of conditional sampling, is proposed by which the particles in 2D/3D images are used without any buffer descriptors.

First, an initial and large model containing new particles is generated. Such particles are not exactly the same ones manifested in the original image but are very similar to the given image. Then, the unrealistic particles, through a mismatch map that is generated from the previous step, are identified. A spherical mesh is generated on each of these particles and is corrected using the morphological information extracted from the input image. The correction is carried out using a Laplacian method. The process of correction is continued until the visiting particle matches the extracted spatial distributions.

Aside from the above new features, one of the other differences of the proposed method in this paper is that the particles are modeled together. In other words, some spatial configurations only occur under specific circumstances and are meaningful when the particles are looked together. Thus, the arrangement, and even the shape, of particles is relevant when are they regenerated with respect to the given settings. For example, most, if not all, of the previous methods model the particles separately. Then, the particles, based on some rules, are packed, which results in ignoring the initial configuration. The proposed method can reproduce the actual intricacy and interlocking of a real sample, and it is also able to fill an arbitrary container with an already dense granular sample.

This paper is arranged as follow: First, the developed method is discussed wherein several features of the proposed algorithm, including grain generation and corrections. Then, the 3D generated models are compared under rigorous statistical tests. Finally, the accuracy of the generated models are compared using flow simulation.

2. Methodology

In this section, the main algorithm cast on a conditional modeling is first introduced. Then, the extracted morphological information, which is required for grain's correction, is described. Finally, the way that the particles are repaired is discussed.

2.1. Computational modeling

The utilized algorithm in this paper is based on a conditional probability inferred from a Markovian property [60–63]. Mathematically speaking, the term Markovian refers to a memoryless property in probability in which the conditional probability of future states only depend on the present state and it does not subject to a sequence of events in past. This concept is used in this paper as the probability of having a void or solid (i.e. grain) phase only depends on the surrounding cells, not the entire simulation space or particles. Furthermore, since the modeling of granular media is considered as a discrete modeling, using the Markovian assumption can alleviate the computational burden of conditional probability. In other words, using the traditional concepts in calculating the conditional probability requires considering all the current and past states for estimating the probability of an event in future, which is computationally expensive.

The modeling occurs on a Cartesian grid **G** with N cells, either in 2D or 3D, and they can be identified with index i. The simulation grid can be of any shape, such as the container of the sample or regular cube/rectangular. An example of such a simulation grid is shown in Fig. 1. Since the investigated problem in this paper is in the form of discrete variables, thus, a discrete variable $z_i\{0,1\}$ is assigned to each cell, which in this case is the phases exist in the initial given image **I**, namely the solid (i.e. particle) or void space. In other words, the final result of the simulation is in the form of 0 and 1, referring to the void and solid spaces, respectively. The input image **I** can be obtained using the tomography methods, which initially is available as 2D/3D grayscale image. The grayscale image requires segmentation to represent the particle as discrete elements. In this study, such a binary image **I** is used as the input data. Thus, the modeling grid can be expressed as $\mathbf{z} = \{z_1,z_2,...,z_i\}$, where z_i indicates the value that is taken by cell N. Then, the joint probability can be written as:

$$\chi(\mathbf{z}) = \chi(z_1)\chi(z_2|z_1)..\chi(z_N|z_{N-1},z_{N-2},...,z_2,z_1). \tag{1}$$

Due to making a Markovian assumption, the conditional probability for z_i depends on small subset, that is the sequential neighborhood of cell i, or $\{\Psi_i\}_{i=1,2,...,N}$. As mentioned, such a neighborhood is composed of the cells around the vising point, which belong to either the void or solid space. Thus, Eq. (1) can be rewritten as:

$$\chi(z_i|z_{i-1},z_{i-2},...,z_2,z_1) = \chi(z_i|\mathbf{z}_{\Psi_i}), \tag{2}$$

where $\mathbf{z}_{\Psi_i}$ represents the cells located in Ψ_i. Therefore, the joint probability can be written as:

$$\chi(\mathbf{z}) = \prod_{i=1}^{N} \chi(z_i|\mathbf{z}_{\Psi_i}). \tag{3}$$

As a result, the above conditional probability requires considering a small subset of $\{\Psi_i\}_{i=1,2,...,N}$.

Computing the equation requires a considerable amount of time if a large neighborhood is used. One, however, can replace such a probability with a distance function presenting the difference between the already simulated points and **I** as follow:

$$\psi(i,j;x,y) = \int_{x=0}^{\mathbf{O}_x-1} \int_{y=0}^{\mathbf{O}_y-1} \mathbf{I}(x+i,y+j)\mathbf{z}_\Psi(x,y)dxdy, \tag{4}$$

where $\mathbf{O}_x$ indicates the overlap of the new location with the previous cells in x direction, which refers to the Markovian assumption used in this paper. Given the previously simulated cells, Eq. (4) gives the best matching location in **I**. For the sake of simplicity, the equations are written in 2D and similar expression can be used in 3D.

Thus far, the main elements of the utilized algorithm have been discussed: (i) the simulation grid **G**, (ii) similarity function, which is used instead of the original conditional probability to expedite the computations, and (iii) overlap region. Therefore, the described computational procedure commences from a corner on the defined simulation grid. Then, the overlap cells, which can contain either void or solid, are extracted and their similarity with the particles in **I** is computed using Eq. (4). Based on the produce similarity map over **I**, a set of candidates is selected and one of them is inserted in the visiting cell. Clearly, the candidates are selected among those that have the highest similarity with the previous pixels, which can be composed of both void and solid phases. The content of the selected candidates depends on the cell values on the overlap regions and the arrangement of particles in the initial pack **I**. Thus, it should be noted that the particles are not simulated individually, but they are considered together as a pattern. Some of the candidate patterns that are selected from a 2D image are shown in Fig. 2. As can be seen, the patterns can contain either a complete void space, a single grain or only a part of the grain. If the latter is selected (based on its similarity with the previous ones in **G**), then, the next candidate is selected in such a way that it completes the already existing partial grain. As will be discussed, some artifacts can occur if a candidate for completing the imperfect grain is not found. In this manner, new particles are created while the original morphology is preserved within the same distribution. The above process continues until the cells are all simulated. Ultimately, an ensemble of particles is generated on the initial simulation grid **G**.