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Quantity and shape modification for random-fractal-based 3D concrete meso-simulation

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ABSTRACT

The importance of the meso-scale analysis of concrete has been a controversial topic. The accuracy and efficiency of numerical modelling directly influence the results and computational cost. In this study, we propose a versatile fractal-geometry-based modelling method that can generate an aggregate model with a known gradation curve. Two numerical meso-model groups generated by the random fractal method are measured and analysed considering the gradation curve, coarse aggregate content, and fractal dimension as evaluation indices. It is verified that the evaluation indices of the numerical models are consistent with the actual ones. Based on sampling statistical analysis, the geometrical homogenization of the meso-model generated by the random fractal method is found to be satisfactory for meso-scale applications. Furthermore, the random fractal method is shown to have low algorithm complexity.

1. Introduction

Understanding the mechanical behaviour of concrete directly influences construction cost and building safety, which are of great significance.

Concrete meso-mechanics can explain the macro-scale mechanical behaviour of concrete. Therefore, it has become the primary focus area in the field of concrete research, yielding important results [1]. There are two main research approaches within the framework of this theory: experimentation and numerical simulation [2]. Compared with experimentation, numerical simulation offers the advantages of low cost, convenient, and accurate data collection, and freedom from experimental restrictions [2]; hence, it has attracted considerable attention.

The numerical meso-model of concrete is a complex system. In general, analysis results of meso-level concrete simulation are influenced by many factors. Herein, we consider two major influencing factors: the geometry and material properties of each component. In this paper, the geometry of concrete and its simulation are discussed in detail.

A numerical simulation usually involves three major steps: (i) creating the aggregate and cement models, (ii) meshing, and (iii) finite element analysis/discrete element analysis [2]. The quality of the concrete mechanical solution depends on the modelling accuracy, i.e., on the first step of the simulation. However, depending on the user's experience, creation of the numerical model is often a time-consuming task [3]. Therefore, it is important to study and discuss the modelling method.

Many researchers have introduced a number of ways to generate the concrete geometrical model. The modelling method typically includes two key procedures. The first procedure is generation of the aggregates, which includes polyhedron generation using either standard Voronoï/Delaunay tessellation [4–7] or a random spatial polygon growth [8,9]. This procedure should follow the principle of keeping each aggregate convex, which is rather difficult. The second procedure is allocation of the aggregate models in the concrete model, which includes the 3D random particle allocation method introduced by Leite [10], the layering disposition method for random aggregate arrangement introduced by Tang [11], and the grid search method based on the background grid, which is combined with meshing [3,9]. This procedure should follow the principles of making the generated concrete numerical model fit actual situations and avoiding the overlapping of aggregates.

The two key procedures described above are combined to obtain a complete concrete modelling algorithm. The main aspects of the modelling algorithm are computational efficiency and model quality. This paper classifies modelling algorithms into three categories. In the first category, random aggregate models are first generated and then allocated in the concrete model sequentially, e.g., the method introduced in [10], which is a traditional method. Based on this method, it is necessary to judge whether the current particle is completely inside the specimen and overlaps previously placed ones before each particle allocation. The complexity of this method is relatively high; the computation time increases with the number of allocated

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aggregates. Algorithms derived from this method include those introduced in [11,12]. In these methods, the judgment of whether the current particle overlaps previous ones is omitted; this improves the computational efficiency considerably but increases the space between aggregates. The first category profoundly influenced concrete meso-modelling methods; for instance, the NIST model was developed to solve the issue of hydration under seals in [13] and the HCSS to simulate percolation [14]. In the second category, the aggregate models are generated and allocated simultaneously, e.g., the method introduced in [9]. Furthermore, some methods combined with meshing do not require the overlapping of aggregates to be judged, thereby saving a significant amount of time and facilitating follow-up work. Qin [3] showed that it is easy to generate irregularly shaped aggregate models using this type of algorithm, and there is usually a difference between the gradations of the numerical model and actual conditions. In the third category, the location and boundaries of the aggregates are first determined and the aggregates are then generated, e.g., the method introduced in [8] and an algorithm based on random fractal theory introduced by us in [17]. According to the random fractal method (RFM), the boundaries of aggregates around an aggregate can be defined simultaneously with the generation of this aggregate. As with the second category of generating algorithms described above, these algorithms save time but provide a lower coarse aggregate content.

Each of the three types of algorithms described above has its advantages and disadvantages. A major advantage of the RFM is that it involves the application of an index (i.e., the fractal dimension of concrete) that can describe the geometrical character of concrete quantitatively. Such quantitative characterization is useful for extending this algorithm, as it can provide a theoretical basis for follow-up meso-mechanical studies. Therefore, in this paper, we present the theory and implementation of quantity and shape modification for three-dimensional (3D) concrete meso-simulation based on the RFM. With the objective of ensuring low algorithm complexity, the region of applicability is extended and an approach for simulating graded aggregates is proposed.

2. Method

2.1. Principal hypotheses and basic algorithm

2.1.1. Principal hypotheses and assumptions

To establish a systematic and complete theory system, and to simplify the simulation methods, three basic hypotheses are introduced in this paper.

Hypothesis 1. *The set of aggregates and cement is a fractal.*

Hypothesis 2. *All the simulated aggregates are convex.*

Hypothesis 3. *There is always a space between any two aggregates.*

Further details with respect to these hypotheses and some corollaries are presented below.

Based on Hypothesis 1, the theories within the theoretical framework of fractal geometry can be applied. Some conclusions concerned with this study are presented in a later section. The possible availability of the fractal effect of aggregates and cement enables us to use a mathematical expression with the fractal dimension to describe the spatial geometry property of the aggregate condition. Furthermore, this hypothesis makes it possible to generate the aggregate simulation model using the fractal method.

Hypothesis 2 helps to accomplish the following two purposes. (i) It limits the change in the aggregate shape in the simulation process and simplifies the simulation process. (ii) It facilitates element meshing in the finite element analysis stage, thereby preventing abnormal element generation as well as stress concentration. Hypothesis 3 prevents the occurrence of aggregate overlap and reduces the amount of computation. This rule is widely used in the meso-simulation of concrete. The three above-mentioned hypotheses influence the methods of theory and simulation in later sections.

2.1.2. Basic generation algorithm

This corollary, obtained from Hypothesis 1, provides the principal rationale for generating the concrete numerical model using RFM.

Corollary 1. *One approach to fractal geometry is to regard two sets as 'the same' if there is a bi-Lipschitz mapping between them.*

In the theory of fractal geometry, the fractal dimension, which is invariant under bi-Lipschitz transformations, is set up to distinguish between sets that are not homeomorphic. Therefore, if two sets have the same fractal dimension, they are considered to be the same [15].

Based on this corollary, the RFM can be expressed essentially as follows: a geometrical pattern to be generated with the same fractal dimension as that of actual concrete, using the iteration-based modelling algorithm, can be considered as the aggregate numerical model.

The fractal dimension of gradation can be estimated using the definition of Hausdorff dimensions, which we briefly introduce as follows. Considering the ratio of each sieving size x_i to the maximum aggregate size x_{max} as the x-coordinate and the value of the mass retained $P(x_i)$ corresponding to the size of each x_i as the y-coordinate, several points can be plotted in a log-log plot. Then, the slope of the straight line fitted to these points can be determined as 3 minus the fractal dimension [17]. The method for ensuring the correspondence between the fractal dimension of the numerical model and that of actual concrete is detailed in Section 2.4.1.

The basic iterate algorithm for generating the fractal pattern can be represented as follows [17]:

1. Set a cell: consider an initial model as a cell. According to the specific purpose, the cell can be a two-dimensional (2D) or 3D pattern. A cell is considered as an auxiliary pattern. An auxiliary pattern is used for convenience and is virtually non-existent. It is drawn temporarily to facilitate the construction of the model; it neither is shown after the process of modelling nor participates in the calculation.
2. Divide the cell: divide the cell into several sub-auxiliary patterns in accordance with a certain rule, ensuring that these sub-auxiliary patterns are closed and convex.
3. Generate the aggregate(s): change the sub-auxiliary graph(s) at the specified location to a real graph; the real graph is treated as the model of an aggregate.
4. Iteration: treat each remaining sub-auxiliary pattern as a new cell, and repeat steps 2 and 3 until the program ends.

In this study, a single performance of steps 2 and 3 is considered as one iteration. A 2D cell, for instance, is treated by the process shown in Fig. 1, in which a cell is closed and convex. The process shown in Fig. 1 is a mathematical and qualitative representation that describes how rock be crushed into aggregate productions. Hence, a possible application of fractal theory may be the simulation of aggregate production.

When the concrete is simulated, a fractal pattern in which a new segment is scaled by a constant ratio is generated. This characteristic resembles the characteristics of a series of sieve sizes that can be approximated as a geometric progression with a common ratio. However, in practice, a single cell cannot meet the demands of a variety of model sizes for two reasons. First, the actual number of aggregates in each sieving level cannot be an exponential function that depends on the sieving size. Second, the maximum grain size in the model generated by the basic algorithm is the edge length of a cell divided by a fixed value.

The first problem can be solved by first calculating the probability that the aggregate appears in the ideal location and then modifying the quantity of aggregates, as described in Section 2.3. The second