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Numerical modelling of ellipsoidal inclusions

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HIGHLIGHTS

- Algorithm for randomly distributing 3D inclusions.
- Employment of real grading curves.
- Effective simulation of different packing densities.
- Novel dislocation procedure.
- Procedure suitable for modelling composite materials.

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ABSTRACT

Within the framework of numerical algorithms for the three-dimensional random packing of granular materials this work presents an innovative formulation for polydispersed ellipsoidal particles, including an overlapping detection algorithm for an optimized simulation of the mesostructure of geomaterials, particularly concrete.

Granular composite cement-based materials can be so reconstructed with adequate precision in terms of grain size distribution. Specifically, the algorithm performance towards the assumed inclusion shape (ellipsoidal or spherical) and degree of regularity (round or irregular) is here discussed. Examples on real grading curves prove that this approach is effective.

The advantages of the proposed method for computational mechanics purposes are also disclosed when properly interfaced with visualization *CAD* (Computer Aided Design) tools.

1. Introduction

The packing density can strongly influence the performance of granular materials like concrete and the costs related to its production. The basic concept of a packing method is to reduce the voids content by studying an optimum mixture of coarse and fine aggregates, so minimizing the amount of the required binder and water in the mix. The packing of a cementitious material depends basically on the aggregates size and shape and on the applied packing method itself. While the first parameter is determined by choosing recommended grading curves and the latter is easily guaranteed by a satisfactory vibration during casting, the second one can not always be optimized since it is strictly related to aggregate availability. He et al. [1] demonstrated for mono-sized particles that polyhedra with larger sphericity can be packed to a higher density. Sphericity is defined as the surface area ratio of a sphere with a particle, equivalent in volume. Xu and Chen [2] reached a similar conclusion for polydispersed ellipsoidal particles. Similarly in 2D, Xu et al. [3] found that, when ellipses slightly deviate from circles, the packing fraction rises to the maximum value, otherwise it decreases.

When numerically modeling concrete at the mesoscopic scale, i.e. at the scale of its constituents, it is significant to reproduce the real particle packing which is related to the w/c ratio and therefore, practically, to concrete workability and final strength.

The packing of spheres was first theoretically and experimentally investigated in [4] for mixes with very large size difference between the fine and coarse particles. Later Stovall et al. [5] developed a model to predict the packing density of multi-sized grain mixtures, including the loosening and wall effects, i.e. taking into account particle interactions and interactions of the particles at the boundaries.

With the advances in computer simulations many works have focused on the development of algorithms for the random

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distribution of non-overlapping particles. In most studies the assumption of spherical aggregates is made for sake of simplicity [6–8], however some works deal with more complex geometries, e.g. Wittmann et al. [9] generated 2D rounded aggregates by using the morphological law developed by Beddow and Meloy [10] and angular aggregates as polygons, of randomly varying number of edges and angles; more recently Wang et al. [11] developed a procedure for generating random aggregate structures for rounded and angular aggregates based on Wittmann's findings but here angular aggregates are generated as polygons with prescribed elongation ratios, rather than just as randomly shaped polygons. Three-dimensional studies involving ellipsoids are reported in [12–15], while Williams and Philipse [16] used spherocylinders to better simulate the elongation of real particles, such as fibers.

As regards the packing algorithm, two are mainly adopted in the scientific literature: the take-and-place method [9,11,17], which consists in randomly positioning a number of particles necessary to satisfy the sieving classes in which the grading curve can be divided, proceeding from large to small particles; and the divide-and-fill method [18], which consists in subdividing the whole domain in 2D or 3D into sub-regions and fill them with grain particles, based on the grading curve and the aggregate fraction. An optimized algorithm to pack very large volumes of spherical entities, enriched by a genetic module, has been more recently developed in [7]: this method is derived from [19] and it is found to significantly improve the speed of convergence of the sequential packing algorithm of spheres. In line with a "parent–child" model, it adaptively shifts and shrinks the search space in the control volume by employing feasible (with satisfied constraints) and infeasible (with unsatisfied constraints) spheres in the population of "children" to find a sphere with maximum radius. By doing so the module can search the free space within a domain to inscribe the maximum-sized spheres among the previously packed ones, in an optimal way.

Within this framework the work proposes an original, mathematically-based formulation for the ellipsoidal particle size distribution within a 3D space and it discusses its performance when spherical inclusions are employed. The method takes inspiration from the divide-and-fill method but it is improved by the introduction of a control step of new concept and implementation, which allows further packing and an optimized use of the free available space. The study is directed towards a three-dimensional modeling of cement-based composite materials at the mesocopic scale in order to manage space discretization in agreement with the Finite Element Method (FEM) and perform numerical analyses in the context of continuum mechanics [20].

2. Grading curves in concrete materials

The size distribution of aggregate particles in concrete can be defined either by means of grading curves or from sieve analyses.

Several types of ideal grading curves can be applied, the most known and acceptable of them is Fuller's curve [21], which is described by a simple equation relating the percentage of aggregates passing through one sieve P_i to the corresponding sieve diameter d_i and the maximum dimension of the aggregates D_{max}:

$$P_i = 100\sqrt{d_i/D_{max}}. \tag{1}$$

It is well known that Fuller's curve gives good results for low-workability mixes. To obtain a better compaction maintaining a good workability, Bolomey's curve [22] is to be preferred. Eq. (1) is modified according to Bolomey into:

$$P_i = A + (100 - A)\sqrt{d_i/D_{max}} \tag{2}$$

where the parameter A accounts for the impact of adding fine particles in the mix and it derives from imposing an arbitrary percentage A at the 80 μm sieve.

In general, grading curves do not consider the geometry of aggregates, but only the maximum diameter and that related to the current passing percentage. However the geometry must play a role in the compaction process which can not be neglected when modeling a mesoscopic structure that resembles the real one.

European standards [23] give some indications on how to determine the shape index of coarse aggregates; the method applies for natural or artificial aggregates, including lightweight aggregates, and it classifies an aggregate according to two main dimensions: the length of a grain L and its thickness E, defined respectively as the maximum and the minimum distance between two parallel planes tangential to the particle surface (Fig. 1). An aspect ratio L/E greater than 3 accounts for *non-cubic* particles and, in this sense, the test leads to the evaluation of the percentage of *cubic* or *non-cubic* grain fractions of a given mix.

If one accepts that, in line with the European standard, the *non-cubic* condition defines the usability limit of aggregates in a mix, particles with ratio $1 \leqslant L/E \leqslant 3$ can be conveniently approximated by ellipsoids more than spheres (for which $L/E = 1$ Fig. 2) and in this range an ellipsoidal representation is still acceptable; it may be not so for higher L/E ratios.

3. Theoretical background

3.1. Ellipsoidal formulation

An ellipsoid surface satisfies the following equation:

$$f(\mathbf{x}) = \frac{x^2}{l_x^2} + \frac{y^2}{l_y^2} + \frac{z^2}{l_z^2} - 1 = 0 \tag{3}$$

where x, y, z are the position vector components of vector: $\mathbf{x} = [x, y, z]^T$ while $\mathbf{l} = [l_x, l_y, l_z]$ are the semidiameters of the ellipses obtained by sectioning the ellipsoids with the coordinate planes (Fig. 3).

Eq. (3) in matrix notation yields [24]:

$$f(\mathbf{x}) = \mathbf{x}^T\mathbf{B}\mathbf{x} \tag{4}$$

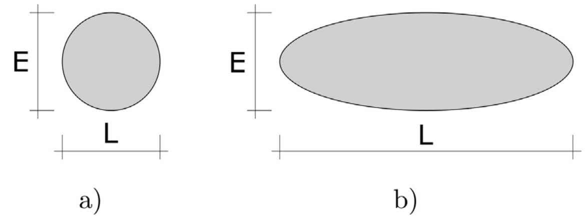

Fig. 1. Aggregate ratio $L/E = 1$; aggregate ratio $L/E = 3$.

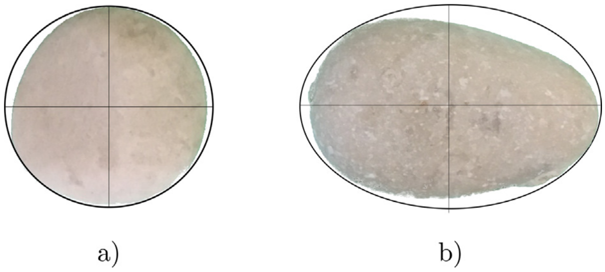

Fig. 2. Spherical aggregate a); ellipsoidal aggregate b).