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Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. I: Theory

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ABSTRACT

This paper deals with the formulation, calibration, and validation of the Lattice Discrete Particle Model (LDPM) suitable for the simulation of the failure behavior of concrete. LDPM simulates concrete at the meso-scale considered to be the length scale of coarse aggregate pieces. LDPM is formulated in the framework of discrete models for which the unknown displacement field is not continuous but only defined at a finite number of points representing the center of aggregate particles. Size and distribution of the particles are obtained according to the actual aggregate size distribution of concrete. Discrete compatibility and equilibrium equations are used to formulate the governing equations of the LDPM computational framework. Particle contact behavior represents the mechanical interaction among adjacent aggregate particles through the embedding mortar. Such interaction is governed by meso-scale constitutive equations simulating meso-scale tensile fracturing with strain-softening, cohesive and frictional shearing, and nonlinear compressive behavior with strain-hardening. The present, Part I, of this two-part study deals with model formulation leaving model calibration and validation to the subsequent Part II.

1. Introduction

Concrete is a heterogeneous material characterized by several length scales of observation ranging from the length scale of crystalline particles of hydrated Portland cement (10^{-9} m) to the macroscopic scale (10^{1} m), at which concrete has been traditionally considered homogeneous. It is now widely recognized that accurate modeling of multiscale materials calls for the adoption of multiscale techniques able to bridge the various scales and to bring to the macroscopic scale the most important effects of lower scale phenomena. In the recent past, publications proposing new multiscale theories have flourished, especially for modeling nano-composite materials and atomistic and molecular systems [23]. The same kind of development has not appeared yet in concrete mechanics literature or in civil engineering in general. The main reason for this can be traced back to the extreme complexity of concrete internal structure and to the unavailability of accurate fine-scale models for concrete.

In the last twenty years, various authors attempted the development of concrete models targeting concrete mini-scale (length scale of 10^{-4} m or less) and meso-scale (length scale 10^{-3} m). The term “mini-scale” was first introduced by Cusatis et al. [18] and is relevant to the description of concrete as a three-phase material: cement paste, aggregate, and interfacial transitional zone, whereas the meso-scale is relevant to the characterization of concrete as two-phase material: mortar and coarse aggregate. It must be noted that some authors use the term “meso-scale” in a wider sense to include the “mini-scale”.

Mini-scale models were proposed by several authors [29,30,10,1,9,33]. Remarkable are the contributions due to Wittmann and coworkers [29] for 2D models, and to Carol and coworkers [12,11,13] for 3D models. They used finite element techniques to model, with different constitutive laws, coarse aggregate pieces, mortar matrix, and an inclusion-matrix interface. This led to very large computational systems characterized by several thousands of degrees of freedom even for the simulation of small specimens. An alternative to the use of finite elements was proposed by Van Mier and coworkers [30] who removed the continuum hypothesis and modeled concrete through a discrete system of beams (lattice). In their approach, lattice meshes were superimposed to digitalized images of the concrete internal structure to assign different material properties to the lattice elements corresponding to the various components (matrix, aggregate, and interface). Along this line, Bolander and coworkers [9,33] formulated a discrete mini-scale model based on the interaction between rigid polyhedral particles obtained though the Voronoi tessellation of the domain. Similar approach was used by Nagai et al. [26] to simulate mortar and

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concrete in a 2D setting. Mini-scale models provide realistic simulations of concrete cracking, coalescence of multiple distribute cracks into localized cracks, and fracture propagation. However, they tend to be computationally intensive, especially for 3D modeling that is required to correctly capture compressive failure and confinement effects.

Computationally less demanding are the meso-scale models [5,16,18] in which the basic material components, whole aggregate pieces and the layer of mortar matrix between them, are modeled through discrete elements (either lattice elements or discrete particles) but are themselves not discretized on a finer scale. Meso-scale models greatly reduce the size of the numerical problems but at the same time can capture the fundamental aspects of material heterogeneity. Meso-scale models have made possible the realistic simulation of both tensile and compressive softening. Preliminary results on the modeling of multiaxial behavior and confinement effects were also achieved by Cusatis et al. [17] and Belheine et al. [7].

The main objective of this article is to discuss a recently developed meso-scale model for concrete, called the Lattice Discrete Particle Model (LDPM). The development of LDPM is a synthesis of two independent research efforts that led to the formulation of the Confinement Shear Lattice (CSL) Model [18,16,17] and the Discrete Particle Model (DPM) [27].

LDPM shares the following features with CSL: (a) it simulates concrete mesostructure by a system of interacting aggregate particles connected by a lattice system that is obtained through a Delaunay tetrahedralization of the aggregate centers; (b) the position of each aggregate piece throughout a given concrete specimen is defined by means of the basic concrete properties and the size distribution of the aggregates; (c) the geometry of the lattice struts connecting adjacent particles is obtained by a three-dimensional domain tessellation defining a set of polyhedral cells each including one aggregate piece; (d) the mechanical interaction between the particles is characterized by both normal and shear stresses; and (e) the meso-scale constitutive behavior is softening for pure tension and shear-tension while it is plastic hardening for pure compression and shear-compression.

LDPM inherited from DPM the Modeling and Analysis of the Response of Structures (MARS) computational environment [28] that includes long range contact capabilities typical of the classical formulation of Discrete Element Methods (DEM) [15]. This feature is particularly important for simulating pervasive failure and fragmentation.

While building on the successful developments of CSL and DPM, LDPM formulation is characterized by a number of new features that greatly enhance its modeling and predictive capabilities. These new features can be summarized as follows:

1. Interaction among the particles is formulated through the analysis of an assemblage of four aggregate pieces whose centers are the vertexes of the Delaunay tetrahedralization. This makes possible the inclusion of volumetric effects in the constitutive law that cannot be taken into account by the two particle interaction used in CSL and DPM.
2. Stresses and strains are defined at each single facet of the polyhedral cells containing the aggregate pieces. Compared to previous formulations, this allows a better stress resolution in the mesostructure, which, in turn, leads to a better representation of meso-scale crack and damage distribution.
3. The constitutive law simulates the most relevant physical phenomena governing concrete damage and failure under tension as well as compression. Compared to the constitutive law used in the previous work [16], the present law provides better modeling and predictive capabilities especially for the macroscopic behavior in compression with confinement effects.
4. The constitutive equations include simple but effective unloading-reloading rules that permit an accurate simulation of concrete response under cyclic loadings.
5. The constitutive equations also include the effect of material compaction and densification due to the effect of high confining pressures.

The present formulation can realistically simulate all aspects of concrete response under quasi-static loading, including tensile and compressive strength, cohesive fracture and size effect, damage in compression, compression-shear behavior with softening at zero or low-confinement and hardening at high confined compression, and strength increase under biaxial loading. This paper (Part I of a two-part study) discusses the details of LDPM formulation and its numerical implementation. Part II will focus on its extensive calibration and validation.

2. Geometrical characterization of concrete mesostructure

The geometrical characterization of concrete mesostructure is based on a four-step procedure that aims at defining (1) the number and size of coarse aggregate pieces (particles); (2) particle position; (3) interparticle connections; and (4) surfaces through which forces are transmitted between adjacent particles. These surfaces will also represent weak locations in the concrete mesostructure, where damage is likely to localize.

2.1. Particle generation

In the first step, particle generation is carried out by assuming that each aggregate piece can be approximated as a sphere. Under this assumption, typical concrete granulometric distributions can be represented by the particle size distribution function (psd) proposed by Stroeven [32]:

$$f(d) = \frac{q d_0^q}{[1-(d_0/d_a)^q] d^{q+1}} \tag{1}$$

where d_a is the maximum aggregate size, and d_0 is the minimum particle size used in the simulations, and q is a material parameter. It must noted here that, in general, $d_0 \neq 0$ to limit the number of degrees of freedom to be solved in the numerical simulations. The above psd can be interpreted as the probability density function (pdf) for the occurrence of a certain diameter d. The cumulative distribution function (cdf) can be then computed as

$$P(d) = \int_{d_0}^{d} f(d)\mathrm{d}d = \frac{1-(d_0/d)^q}{1-(d_0/d_a)^q} \tag{2}$$

It can be shown [32] that the psd in Eq. (1) is associated with a sieve curve (percentage of aggregate by weight retained by a sieve of characteristic size d) in the form

$$F(d) = \left(\frac{d}{d_a}\right)^{n_F} \tag{3}$$

where $n_F = 3 - q$. For $q = 2.5$ ($n_F = 0.5$), Eq. (3) corresponds to the classical Fuller curve which for its optimal packing properties, is extensively used in concrete technology [24].

For a given cement content c, water-to-cement ratio w/c, specimen volume V, maximum aggregate size d_a, and minimum particle size d_0 (which governs the resolution of the model), particles to be placed inside the volume can be obtained as follows:

1. Compute aggregate volume fraction as $v_a = 1 - c/\rho_c - w/\rho_w - v_{air}$, where $w = (w/c)c$ is the water mass content per unit volume of concrete, $\rho_c = 3150\ \mathrm{kg/m^3}$ is the mass density