Inherent Variability of Lattice Discrete Particle Models Caused by Particle Placement Strategies

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Abstract: The paper aims at characterizing the influence of particle placement and clustering in lattice discrete particle models (LDPM) on structural response. More specifically, the meso-structural features are mimicked by the proposed particle placement schemes for LDPM, which are no longer independent and random but are correlated to prescribed fields. The study is based on high-dimensional Monte Carlo (MC) LDPM simulations of three classical concrete tests in which the inherent variability and production process are represented by the proposed particle placement schemes with varying parameters, and constant material and composition properties.

Keywords: Lattice Discrete Particle Model; particle placement; Monte Carlo; structural response.

1 Introduction

Many materials used in civil engineering are heterogeneous and characterized by several length scales, e.g. concrete, fibre reinforced, or particulate filled composites. Various numerical models have been developed to simulate miscellaneous material behaviour. Providing the quasi-brittle materials are in focus, two different groups of approaches have been formulated and developed throughout the years: (1) the discrete fracture formulation, such as cohesive (fictitious) crack model and finite elements (FE) with discontinuity (see [1, 2]), that are not considered in this study; (2) the models with distributed cracking/damage using continuum finite elements and discrete elements such as random lattice or particle model. In the latter approach, many constitutive models have been developed over the years to describe the behaviour of concrete: based on the concepts of plasticity [3], damage mechanics [4], a combination of both, or fracture mechanics [5]. They are typically formulated in tensorial (classical continuum-based theory) or vectorial form (e.g., microplane theory, discrete particle models) [6].

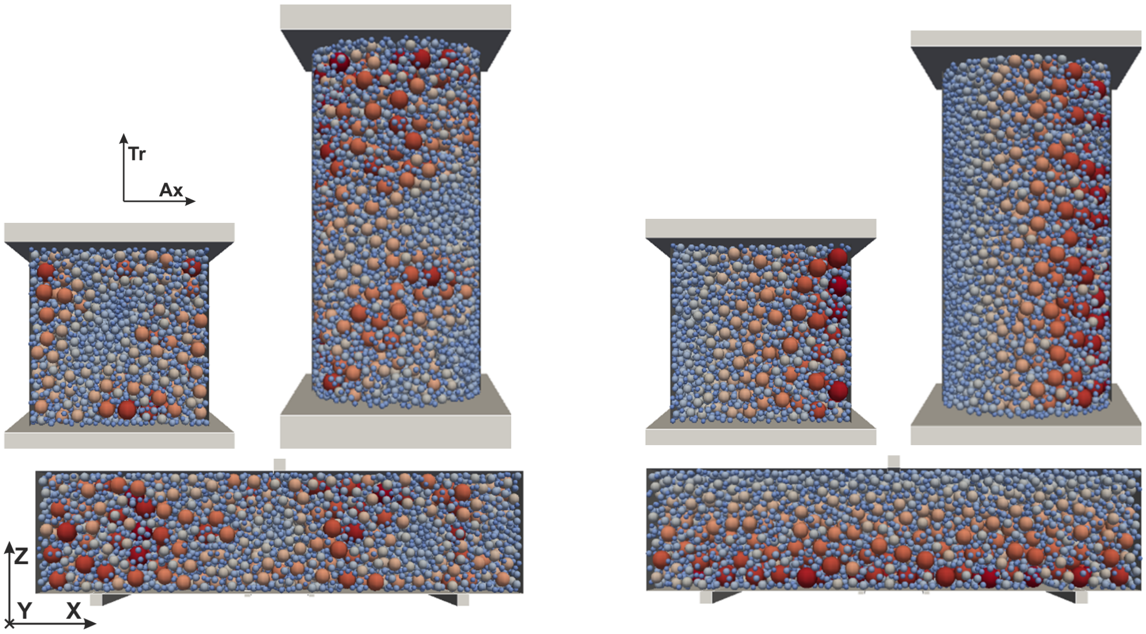
In this paper, we put our attention on the discrete particle model, more specifically Lattice Discrete Particle Model (LDPM) introduced by Cusatis et al. [7]. The LDPM material model response is dependent on particle distribution, and thus multiple simulations are needed to provide credible results [8]. This variability is often considered similar to experimental scatter. However, the numerical model scatter is usually much smaller than the experimentally observed. Therefore, the particle placement influence and its affect on the response scatter is investigated in the paper.

2 Lattice Discrete Particle Model (LDPM)

A well-established member of the discrete framework, the lattice discrete particle model (LDPM), has been extensively calibrated and validated. It has shown superior capabilities in reproducing and predicting concrete behaviour in many practically relevant applications [8, 9, 10]. It simulates the mesostructure of concrete by a three-dimensional (3D) assemblage of particles generated randomly according to a given grain size distribution (Fuller curve). After the particles are randomly placed in the concrete domain from the biggest to the smallest, the lattice mesh is generated, connecting the centres of the spheres. The topology of the interaction among particles is obtained by the Delaunay tetrahedralisation and a tessellation of the domain; for more details see [7]. Displacements and rotations of such adjacent particles form the discrete compatibility equations in terms of rigid body kinematics. At each cell facet, the mesoscale constitutive law is formulated such that it simulates cohesive fracture, compaction due to pore collapse, frictional slip and rate effect. For every single particle, equilibrium equations are finally formulated.

3 Particle Placement

The numerical models of classical concrete experiments are introduced, i.e. cubes and cylinders loaded in compression and unnotched beams loaded in three-point bending. As already mentioned above, the internal structure of the material is modelled through discrete elements to capture the fundamental aspects of heterogeneity. Essential inputs for the models are the maximum and minimum aggregate sizes which are used for the particle size generation based on the classical Fuller curve. The higher bound of the sieve curve is defined by the maximum aggregate size (d_a) while the minimum aggregate size (d_0) defines its arbitrary lower cut-off, i.e. the diameter under which no particles are discretely generated and placed. Thus, the minimum aggregate size affects the refinement of the discrete mesh and consequently also the computational cost. In the original formulation, a statistically isotropic random mesostructure is utilized to create the numerical models. In the present paper new placement procedure is introduced to mimic the segregation or clustering of large particles in specimens caused by the casting process. More specifically, gradient-based generation is utilized in the paper. The response scatter of these approaches are compared, and conclusions are drawn. In the paper, the random and gradient field-based generations are studied (Fig. 1).



(a) random field

(b) gradient field

Fig. 1: Visual representation of particle placement for compression and three-point bending tests.

Particle generation governed by a field is a modified version of a standard geometrical characterization of the concrete mesostructure presented in [7]. In the present study, the generated mesostructure has to follow both the particle distribution curve and the distribution of a given field, e.g., random, directional. In the first step, particles represented by spheres are generated following the defined concrete granulometric distribution. The main difference between the standard and the new procedure lies in the particle placement strategy. The particle centres are positioned throughout the specimen volume one by one (from the largest to the smallest). Assuming

Tab. 1: Results for the three-point bending tests. The COV is expressed in $\%$.

Property	IRPP	PGGF		
		Z^-	Z^-	Y^+
L@P [MPa]	11.1$\pm$2.8%	11.4$\pm$2.0%	11.0$\pm$1.7%	11.2$\pm$1.8%
D@P [-]	0.039$\pm$4.5%	0.040$\pm$3.3%	0.038$\pm$2.7%	0.039$\pm$2.9%

Tab. 2: Results for the cylinder compression tests. The COV is expressed in $\%$.

Property	IRPP	PGGF	
		A_x	T_r
L@P [kN]	21.5$\pm$0.4%	20.8$\pm$0.7%	21.2$\pm$0.5%
D@P [μm]	1.2$\pm$1.2%	1.1$\pm$1.0%	1.2$\pm$1.7%

that N_0 particles have to be placed, N_0 random particle positions are generated, and the intensity for each of them is evaluated based on the prescribed field. The positions are then ordered following the given intensity (from the highest to the lowest), and the position with the highest intensity is assigned to the largest particle. The largest particle is then placed at this position (assuming that it does not cross the domain's border), and both the particle and the position are deleted from their lists. Next, the new position with the highest intensity is utilized to position the new largest particle (previously second in the particle list). If there is no conflict with the previously placed particle(s) and the domain's boundary, the particle is placed and again deleted from the list. However, suppose it exceeds the domain boundary or overlaps with the previously placed particle(s). In that case, this position is discarded, a new random position is generated, and its intensity is evaluated. Then the positions are again ordered based on the given intensity, and the particle placing procedure continues as described before. To minimize the geometrical bias of the discretization, a minimum distance between two adjacent particles is defined as $\delta_s\,(r_1 + r_2)$, where $r_{1,2}$ stand for the radii of the particles and $\delta_s \geq 0$ is the non-dimensional scaling parameter. The utilized minimum distance rule allows a smaller distance between small and large particles compared to the distance between two large particles. $\delta_s = 0.1$ is utilized in the current study.

4 Results

Along with simulations in which the particle generation is governed by a field (PGGF), the independent and random particle placement (IRPP) simulations were run for direct comparison. In all cases, 20 repetitions per specimen configuration were run. The results used in the comparison are: (a) the mean stress or the mean force at peak (mean L@P); (b) the mean strain or the mean displacement at peak (mean D@P) for beams and compression specimens, respectively. Also, their coefficients of variations were computed for the comparison.

Tables 1-3 show the IRPP and PGGF results for the three geometries and also different orientations of gradient fields. The results reveal only a slight change in the results and scatter compared to IRPP if the PGGF based generation is utilized.

Tab. 3: Results for the cube compression tests. The COV is expressed in $\%$.

Property	IRPP	PGGF	
		A_x	T_r
L@P [kN]	26.2$\pm$0.6%	25.8$\pm$0.6%	26.0$\pm$0.7%
D@P [μm]	1.7$\pm$3.6%	2.9$\pm$1.0%	3.5$\pm$1.7%

5 Conclusion

A spatial variability package for the LDPM has been presented, including two new abstraction levels for the discrete framework where an initial random field governs material characterization and particle generation. The presented work is the first step of a more extensive investigation. Modelling concepts for different sources of spatial variability in materials (concrete) are being investigated, including spatially variable material property fields. In order to study the pure effects of the particle generation process governed by random or gradient-based fields, the material properties have been kept constant for all of the presented analyses.

Based on the presented results, the following conclusions can be drawn:

- Directional effects, mimicking production processes (concrete casting) and represented by gradient-based fields, may slightly affect both the mean values of force at peak, displacement at peak, and their respective coefficients of variation of the response;
- Correlated spatial variability models (random fields) governing the particle generation process moderately influence the COV of the response compared to the independent and random generation of particles;
- The investigated particle placement schemes with constant material and composition properties enhance the realism of the simulations but are insufficient to reproduce the experimental scatter.

Acknowledgement

The financial support provided by the GAČR grant No. 21-28525S is gratefully acknowledged.

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