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Circular representative volume element for discrete model of concrete

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1. Introduction

Representative volume element (RVE) is a concept used in homogenization schemes, which potentially allows the reduction of computational costs of highly detailed simulations [6]. In essence, it is a small-scale (micro or mesoscale) model, which statistically represents a material used for a macroscale simulation. In a computational scheme (for example the Finite Element Method), it acts as a constitutive function substitution: An RVE is attached to an integration point, loaded by proper displacement or traction and its response is obtained. Subsequently, the results are used in the macroscale calculations [5].

Loading, whether displacement or traction, may be applied on the RVE in multiple ways, however, it has been shown that periodic boundary conditions are the most advantageous since the response they produce is the most realistic one [8]. RVE in combination with periodic boundary conditions is overwhelmingly used only for elastic response [6]. When applied to non-linear scenarios, for example a strain softening material with heterogenities, whose post-peak behavior is characterized by fracture, its use is also possible, albeit its statistical representativeness is questionable. It requires extensive modification to the original equations defining the boundary conditions and some transformation (rotation, translation) of the coordinate system so that a crack may emerge in an arbitrary direction. Apart from leading to complex implementations, such modifications inevitably add additional computational costs [2, 8–10].

One of the possible solutions proposed in literature, which builds on the concept of an RVE used in conjunction with periodic boundary conditions, is to substitute the conventionally used square / cubic RVE by a circular / spherical one [7,9]. Such solution potentially offers seamless rotation of the coordinate system so that periodic boundary conditions allow the formation of a crack in arbitrary direction.

The present contribution is part of a larger effort to formulate a circular RVE formed by a lattice discrete particle model (LDPM) [3, 4] which could also account for a post peak strain softening behavior. It is concerned with the generation of a circular RVE geometry mimicking discrete setting which enables periodic placement of particles. We presume that the use of a discrete model does not allow the splitting of a particle and therefore necessarily leads to the generation of a irregular boundary. In the first part, the formation of a continuous circular RVE described in literature is shown. Subsequently a formation of a discrete circular RVE is mimicked by altering the boundary of a RVE. It is shown that this may lead to spurious strains being introduced into the RVE response. Possible modifications to the generation procedure are proposed and tested.

2. Circular RVE geometry generation

In an RVE formulation, periodic boundary conditions are prescribed for each opposing couple of nodes on the surface of an RVE. Each couple of points is allowed the same displacement and rotation. According to [7], the only requirement to which the shape of an RVE is subjected is that of opposing surface normals for each couple of nodes: $n^+ = -n^-$.

Upholding the periodicity of a material, geometry generation is according to [9] done by placing a periodic image of a particle with center (r, θ, ϕ) to a particle of the same diameter with center $(r - D, \theta, \phi)$, where D is the diameter of the RVE (Fig. 1a). In case of a circular RVE with particles created by continuous model, such requirement is naturally fulfilled, because the heterogeneities may be split and thus the surface of a RVE is kept regular (Fig. 1b). In the case of a discrete model with physical discretization [1], such split of particles is not possible by the nature of the model, hence the periodicity of the material must be upheld by allowing irregular boundary (Fig. 1c).



Fig. 1. (a) Geometry generation of a circular RVE with periodically placed particles, (b) a schematic boundary of a continuous RVE and (c) a schematic boundary of a discrete RVE

2.1 Simulations

Both of the scenarios described above have been tested in simulations, in order to asses its performance in elastic regime. To see the effect of the boundary manipulation, only the position of one node couple was altered (Figs. 1b and 1c). Elastic material of given parameters was used. No heterogeneities were incorporated. Periodic boundary conditions are applied to the opposing node couples. An in-house Finite Element Method preprocessor and solver, named OAS (Open Academic Solver), was used. The RVEs are loaded by uniaxial tension applied in the x direction $\varepsilon = \{\varepsilon_{xx} \ 0 \ 0\}^T$. Strain fields of the loaded RVEs are shown in Fig. 2.

The RVEs were both loaded by a strain $\varepsilon_x = 0.001$. The strain field of a RVE with regular boundary shows constant distribution of strains, with magnitude being equal to that of the applied loading. On the contrary, the RVE with irregular boundary shows that by the irregularities, strain magnitude differs by as much as 50 %, ranging up to 0.0015 magnitude. The difference lowers by decreases meshing of the RVE, but it remains present.

Upon closer inspection, the second RVE with irregular boundary does not abide by the condition of opposing normals. Fig. 3a illustrates the mismatch in supposedly parallel boundary segments. Segments of the same style (either solid or dotted line) are centrally symmetric and therefore should be parallel to allow for opposing normals. Clearly, that is not the case. To allow the segments to be parallel, the boundary needs to be changed in a centrally symmetric manner as well (Fig. 3b and 3c).

Results of the simulations performed in the same manner as described at the beginning of this subsection are shown in Fig. 4. The results show that by generating the geometry in a



Fig. 2. (a) Scheme of the loaded circular RVE, (b) strain field (magnitude) of a circular RVE with regular boundary, (c) strain field of a circular RVE with irregular boundary (mimicking discrete RVE)



Fig. 3. Part of the RVE boundary which are joined to the deviated node of the boundary. Lines of the same pattern should be parallel to satisfy the opposing normals equation: (a) not parallel lines of the RVE generated based on the procedure used in [7,9], (b) and (c) suggested modifications to the geometry to maintain constant distribution of strains



Fig. 4. (a) Strain distribution of the first geometry generation with not parallel boundary segments, (b) and (c) results obtained by a centrally symmetric geometry generation

centrally-symmetric manner (Fig. 3b and c), the distribution of strains is equivalent to that of the RVE with regular boundary.

3. Conclusion

It was shown to what extent geometry generation may influence the distribution of stresses in a circular RVE upon which periodic boundary conditions are applied. Following the procedure suggested for the geometry generation of a continuous RVE, the boundary irregularity oriented inward to the RVE behaves as a concentrator, raising the strain magnitude by as much as 50 %.

The strains are lower by the boundary distorted outside of the RVE. The phenomena may be attributed to the effect of periodic boundary conditions, which are in this case applied in a centrally symmetric manner to a non-symmetric node pair.

However, by distorting the boundary in a centrally symmetric manner, that is in the same direction with respect to the centroid of the RVE, the strain distribution is constant as in the case of the regular RVE. Although successful for the present analysis, it is left upon further discussion whether such a geometry generation produces geometrically periodic sample of a material, upholding the original concept of a representative volume element.

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