CIRCULAR REPRESENTATIVE VOLUME ELEMENT FOR HOMOGENIZATION OF DISCRETE MODEL OF CONCRETE

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Abstract
The contribution presents initial results obtained by employing a circular representative volume element (RVE) for the homogenization of a discrete model of concrete. Based on initial research, circular RVE might be a promising alternative to the classical square one (for 2D problems), especially considering its use in conjunction with periodic boundary conditions after strain localization in the material. The contribution shows the behaviour of the circular RVE in elastic loading and compares it to the results obtained by the usually used square RVE.

Keywords
Representative volume element, homogenization, Lattice Discrete Particle Model, elasticity

1 INTRODUCTION

In recent years, discrete models have started to gain popularity because of their ability to naturally model the inner structure of heterogeneous materials. Such capabilities do not come without certain associated costs, such as increased computational demands [1].

To exploit the advantages of detailed physical models, a mathematical method called homogenization is often used (see an example of such an approach in Ref. [2]). It essentially allows the transformation of a computational scheme into a multiscale computational framework, so that detailed, computationally demanding models are used to substitute constitutive relations in the original framework. An example of the Finite Element Method (FEM) framework used on the macroscale complemented by a detailed mesoscale/microscale model attached at an integration point can be seen in Fig. 1.

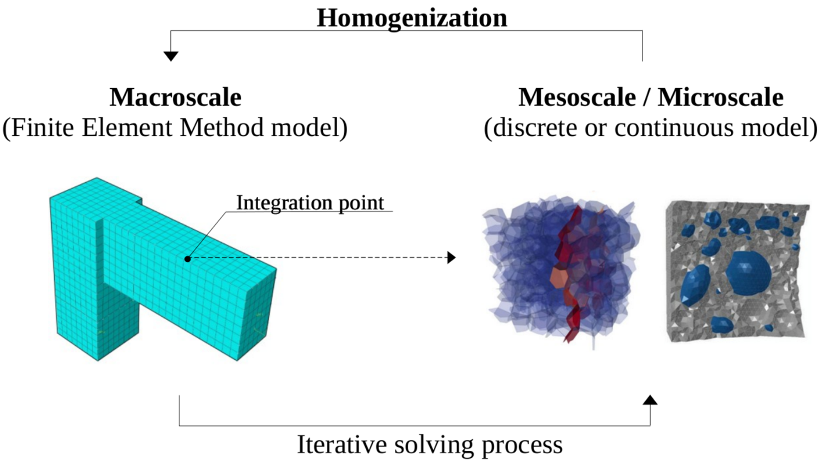

Fig. 1 Basic multiscale computational scheme. Figure of the discrete model has been generated by in-house software; other Figures were taken from [1].

The model used on the mesoscale/microscale level is referred to as the Representative Volume Element (RVE). It is a statistically representative sample of the material, significantly smaller than the macroscopic structure to which it is attached at each integration point of the meshed macroscale domain. In each step, the RVE is loaded by given strains and its response in the form of the stress tensor is calculated and returned to the macroscale [2].

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Based on the response one can also compute effective macroscale material properties. Because the detailed model is not used for the whole macroscale structure, the calculations may be potentially significantly less demanding.

Commonly, square (2D) or cubic (3D) RVE are being employed in elastic regimes. Extension to post-peak behaviour of heterogeneous materials have also been successfully implemented [3], [4], however, several problematic aspects which stem from the occurrence of a localization band. One of the suggested approaches potentially at least partially eliminating the problematic aspects is the use of a circular RVE seen in Refs. [5], [6].

The presented contribution forms part of an ongoing effort to formulate an RVE of a discrete mesoscale model of concrete (the Lattice Discrete Particle Model - LDPM [7]), which could later be used for homogenization in post-peak regime with localized strains as well. After the introduction of the RVE formulation, both square and circular RVEs were analysed and employed to determine effective elastic material parameters. Results obtained on the squared RVE served as a benchmark based on which the performance of the circular RVE was assessed.

2 REPRESENTATIVE VOLUME ELEMENT

A crucial stepping stone in formulating a multiscale computational scheme was the definition of the RVE along with the boundary conditions. Commonly, a square form of the RVE is used in connection with periodic boundary conditions (PBC), which have been shown to provide the most consistent results in terms of RVE stiffness [4]. In principle, the boundary conditions divide opposing surface nodes into two groups, positive and negative, and define the relationship between their displacements $\boldsymbol{u}^+$ and $\boldsymbol{u}^-$, and rotations $\boldsymbol{\theta}^+$ and $\boldsymbol{\theta}^-$ with the help of a macroscale strain tensor $\boldsymbol{\varepsilon}^M$ and the difference between their positions $\boldsymbol{x}^+ - \boldsymbol{x}^-$ as [6]:

$$\boldsymbol{u}^+ = \boldsymbol{u}^- + \varepsilon^M . (\boldsymbol{x}^+ - \boldsymbol{x}^-) \tag{1}$$

$$\boldsymbol{\theta}^+ = \boldsymbol{\theta}^- \tag{2}$$

On a square geometry, opposing node couples $\boldsymbol{x}^+$ and $\boldsymbol{x}^-$ lie on the opposite sides of the square periodically. The constraint is thus applied in two directions. On a circular RVE, the constraint is also applied on opposing nodes, however, it is centrally symmetrical concerning the centre of the RVE. Both cases are shown in Fig. 2, on a geometry generated for the analysis described further on. A detailed account of the geometry formulation may be found in [2].

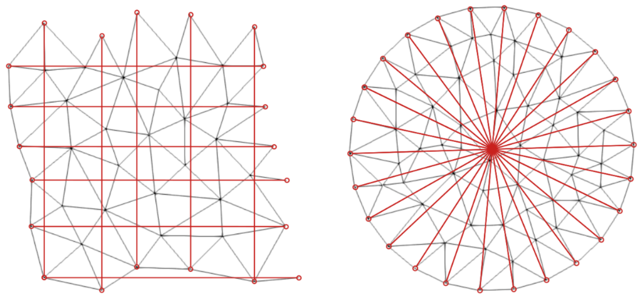

Fig. 2 Periodic boundary conditions applied by a constraint to opposing nodes. Red lines show the pairs of periodic nodes with degrees of freedom bound by equations (1) and (2).

There is a clear difference visible from the two examples in terms of a boundary between the RVEs. The square RVE is formulated in a periodic manner where the periodicity is characterized by irregular boundaries so that the RVE may periodically fill the space of the media. In addition, such a boundary does not impose a wall effect [8], [9] by allowing for irregularity and thus mimicking elements crossing the boundary of a regular square. On the contrary, the circular RVE has a regular boundary.

The regular boundary geometry has been chosen for the circular RVE because PBC may be applied only under the condition that there are opposing norms to the surface in the node couples: $n^+ = n^-$ [5]. This may be achieved either by a regular boundary or by allowing opposing nodes to be disrupted by the same distance from the centre. Neither option offers the perfect periodicity which is achieved by square RVE so regular circular geometry has been chosen for the initial analysis.

It should be noted that this issue is specific to the use of a discrete model. In continuous models, heterogeneities or cavities may be split to partly occur on opposite sides of the RVE so the boundary may be kept regular while maintaining no wall effect.

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3 SQUARE AND CIRCULAR RVE COMPARISON

The aim of the present analysis was to compare the performance and convergence of the circular RVE to the square one. The analysis was done in elastic regime only by numerically obtaining macroscale material parameters Young's modulus E and Poisson's ratio v from the mesoscale RVE response for both square and circular RVE and comparing them. The present section describes the procedure in detail. Unless stated otherwise, variables were considered in the corresponding system of units.

Both RVEs of LDPM geometry (specifics are described in Ref. [9]) are loaded by a strain tensor with one unit component either ε_{xx}, ε_{yy} or γ_{xy}. The strain is applied to RVEs of different sizes, while the criteria for the similarity between the square and the circular RVEs is the RVE area (not the number of elements or number of boundary nodes). RVEs of following areas were considered: A_1 = 0.005 m^2, A_2 = 0.02 m^2, A_3 = 0.08 m^2, A_4 = 0.32 m^2, A_5 = 1.08 m^2. 50 geometries were generated per area so that a representative amount of data was obtained. Each of the geometries was separately loaded by the unit strain so that corresponding stress was obtained (σ_{xx}, σ_{yy} and τ_{xy} per size and geometry). Subsequently, the stress obtained for different geometry realizations corresponding to the same area size was averaged and a numerical material matrix $\boldsymbol{M}^{num}$ describing the response of a square or circular RVE of a certain area in all directions was assembled. Analytical material matrix $\boldsymbol{M}^{an}(E, v)$ (equation (3)) was obtained based on effective Young's modulus E and Poisson's ratio v.

Plane stress state was considered when assembling the matrix

$$\boldsymbol{M}^{an}(E,\nu) = \frac{E}{1-\nu^2}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix}. \quad (3)$$

An optimization algorithm was used to minimize an objective function $\boldsymbol{\Phi}$ (equation (4)) by an open-source optimization module from the SciPy library [10] in order to obtain numerical macroscale parameters for each RVE size and geometry.

$$\boldsymbol{\Phi} = \sqrt{\frac{\sum_i \sum_j \left(M_{i,j}^{num} - M_{i,j}^{an}\right)^2}{\sum_i \sum_j \left(M_{i,j}^{num}\right)^2}} \quad (4)$$

Results

Fig. 3 and Fig. 4 summarize results obtained by the previously described analysis. Both macroscale parameters E and v were compared for square and circular RVEs of different sizes. 50 geometry realizations were tested, hence each curve shows the mean and standard deviation of the obtained values.

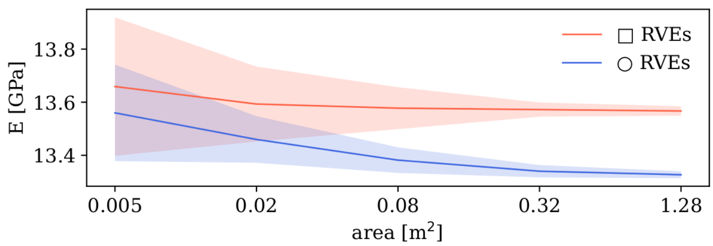

Fig. 3 Resulting Young’s modulus E obtained for various RVE sizes of both shapes.

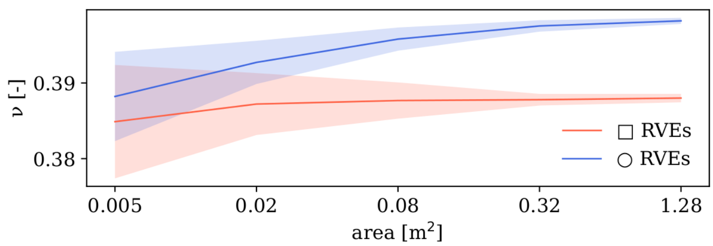

Fig. 4 Resulting Poisson’s ratio v obtained for various RVE sizes of both shapes.

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4 DISCUSSION

Results show a certain discrepancy between the obtained values. In the case of Young's modulus E of the square RVE, the value clearly converges to $E = 13.6$ GPa. The mean value tends to differ only marginally for the smallest area, which is also characterized by the greatest standard deviation. On the contrary, the same quantity obtained from the circular RVE shows the finalmean value to be about $E = 13.4$ GPa, the difference is approximately 1.5%. It is worth noting that the mean value decreases with the increased area of the RVE which is caused by the wall effect due to regular boundary. As in the case of the square RVE, the standard deviation decreases with increased RVE area.

It is presumed, that the final value for the circular RVE is converged (also given the small standard deviation) because the RVE reaches such size that the wall effect [9], [8] is no longer prominent. Although the circular RVE has a regular boundary and thus simulates being a sample by itself (wall effect is present), at the highest size it exhibits the same behaviour as if it was cut from a larger volume (no wall effect). It is worth noting that it is impossible to produce a perfectly periodic circular RVE so a certain substitution will be designed.

The resulting Poisson's ratio which is displayed in Fig. 4 shows similar trends, only the mean value of ν obtained for circular RVE increases with increased RVE size. For both RVE shapes the standard deviation decreases with increased RVE area as expected. Poisson's coefficient of the square RVE converges to $\nu = 0.386$ while for circular RVE the final value is $\nu = 0.395$, the difference concerning the square RVE value being 2.3%. The difference concerning the square RVE's characteristics may be considered significant since the response is expected to be the same.

The opposing trend for both macroscale material characteristics in the circular RVE results suggests that the values tend to compensate for each other. Also, there are more surface node couples in the circular RVE than in the square RVE of the same area (see Fig. 2), restricting the RVE in multiple directions, possibly causing the compensation of a higher Poisson's coefficient which is compensated for by a lower modulus of elasticity.

To confirm the hypothesis, a similar analysis will be run in the future with Poisson's ratio set to 0. This should eliminate the supposedly compensating behaviour since the effect of lateral contraction will not be present at all, and the resulting values of Young's modulus should be the same.

5 CONCLUSIONS

After introducing the general framework of multiscale simulations along with their benefits, the representative volume element has been introduced as the cornerstone of such computational schemes. Two types of RVEs have been defined: (i) a square RVE, commonly used for the purpose, and (ii) a circular RVE, introduced to potentially compensate for certain disadvantages of the square RVE in inelastic calculations.

An analysis has been performed in order to assess the performance of the different RVE in comparison to square one. Only the elastic regime was considered. RVEs of five different areas were considered while 50 realizations were generated per area for each RVE shape. After obtaining the mesoscale (stress) response of the RVEs, an optimization algorithm was used to calculate macroscale material parameters. Finally, the macroscale parameters were compared. Differences in the results of the circular RVE to the square RV were observed. Possible causes for the discrepancy were discussed, however, further research will have to be conducted to draw conclusions.

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