MULTISCALE MODELLING AND REPRESENTATIVE VOLUMES:
LINEAR–ELASTICITY AND SOFTENING

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ABSTRACT
In order to incorporate the heterogeneous micro- or mesostructure of materials, the multiscale modell-  
ing technique seems to be an adequate analysis tool. Here, the multiscale frame is analysed as a  
macro-meso straight forward routine. The question of the size of the meso-level is analysed on the  
basis of the representative volume element (RVE) concept. For this purpose a procedure for the RVE  
size determination was proposed. The two issues of the RVE size determination and the multiscale  
routine have been analysed in the linear-elastic and softening regimes.

1 INTRODUCTION
For the solution of mechanical problems the multiscale technique (Fish et all [1], Feyel [2], Kouznet-  
ssova et al. [3], [4], Gitman et al. [5], [6] etc.) is used to transfer data between different scales. One  
way to perform a multiscale analysis is as follows: the problem is solved on the highest (macro) level,  
where at each macro-level integration point a meso-level analysis is performed. Next, the results of  
the meso-level investigation are averaged through homogenisation techniques and the results of the  
macro-level analysis are corrected. In other words, a two-scale scheme is introduced to describe the  
structure on macro-level taking into account information from the meso-level. The material on the  
macro-level is considered as homogeneous while at the meso-level the material is heterogeneous.  

In a multiscale technique, an apparent question is what the dimensions should be of the meso-  
level sample that is considered. The size of the meso-level sample is defined by means of a repre-  
sentative volume element (RVE).

The aims of this paper are twofold. Firstly, a procedure of RVE size determination is presented  
and analysed for the cases of linear elasticity and softening. Secondly, a multiscale analysis using  
the results of an RVE study is performed.

2 RVE SIZE DETERMINATION
The problem of the RVE size determination is a key issue in the multiscale routine and needs a  
detailed investigation. The Representative Volume Element (RVE) is widely used in nowadays  
mechanics (Audin et al. [7], Ashihmin and Povyshev [8], Behrens et al. [9], Fraldi and Guarracino  
[10]). Several attempts have been made in literature to develop a procedure to determine the rep-  
sresentative size. Drugan and Willis [11] proposed the quantitative estimates of minimum RVE size  
for elastic composites and also Borbely et al. [12], Bulsara et al. [13], Ashihmin and Povyshev [8]  
suggest a way to define the size of the RVE. An objective method to determine the size of the RVE  
was proposed in Gitman et al. [5]. A short overview of this method is presented in the following  
section.
2.1 Method description

The method is based on the statistical analysis of the numerical experiments performed on several different samples. The heterogeneous material is assumed to consist of matrix, aggregates and interfacial transition zone. Three different aggregates densities (volume ratio) were considered; for each of them four different sample sizes were analysed with the help of five different realisations (redistribution, repositioning of the aggregates), thus 60 numerical tests have been performed. Then, the results were analysed with the help of the Chi-square criterion:

\[
\chi^2 = \sum_{i=1}^{n} \frac{(\sigma_i - <\sigma>)^2}{<\sigma>}
\]

where \(\sigma_i\) being the parameter of interest, representing the average value of the stress in the current unit cell, \(<\sigma>\) is the average of \(\sigma_i\), and \(n\) is the number of realisations for the current size.

2.2 Results

Tension tests (figure 1-a) were performed on the samples, and two cases were studied: a linear-elastic material and a softening material. Softening material behaviour was described using the elasticity based gradient damage model (Lemaitre [14], Peerlings [15], Simone [16]):

\[
\sigma = (1 - \omega)D\varepsilon
\]

where \(\sigma\) and \(\varepsilon\) are stresses and strains respectively, \(D\) is the matrix of elastic stiffness (different for each component of the material) and \(\omega\) is historically dependent strain based softening damage evolution law.

**Linear elasticity** Results corresponding to the linear-elastic case are presented in figure (1-b,c). In figure (1-b), Chi-square values for different aggregate densities and different sizes are presented, together with the table value, which was found according to the prescribed accuracy (95 %) and the number of numerical tests performed (five realisation for each aggregate density and each size). Figure (1-c), derived from figure (1-b), shows the dependence of the RVE size from the aggregate density. It should be noted, that the range of aggregates sizes was the same for the complete series.

**Softening** Results corresponding to the softening case are presented in figure (2-a). The stress-strain diagrams for the different sizes are plotted together in order to give an overview of the material behaviour depending on the size of the sample. It can be observed that in the post-peak regime a bigger sample size results in a more brittle response (steeper slope).
In order to be more precise, figure (2) is showing the statistical analysis (mathematical expectation and standard deviation) of the slopes in two points: the first in the linear-elastic part and the second in the softening part. It is observed that in spite of a good converging pattern with the size values of the standard deviation, the mathematical expectation in the softening case grows with increasing size. In the linear-elastic case both mathematical expectation and standard deviation remain practically constant with increasing size.

In the case of softening it is not possible to find a size, which is representative. In contrast, with increasing sample size the material behaves more and more brittle. Mesh size dependence on this scale is excluded by using a higher-order continuum damage formulation. This supports the conclusion, that in case of softening material behaviour, a representative volume cannot be found.

3 MULTISCALE PROCEDURE. RESULTS

On the macro level in the multiscale computation (figure 3), the material is considered to be homogeneous with an imperfection in the middle of the macro-structure (10% reduction in the cross-section). Instead of a constitutive relation on the macro-level, an averaged response from the meso-level has been used. On the meso-level, material is considered to be heterogeneous: matrix with inclusions, surrounded with an interfacial transition zone. Each of these components has its own mechanical properties.

These results (in the same way as it has been done for the RVE size determination) were analysed in two regimes: linear-elasticity and softening. In both of those regimes the issues of meso-size dependence was studied.
As it was mentioned above, two different sizes of the meso-level have been used in the multiscale routine. The difference between the response of the macro-level on changing the size of the meso-level in the linear-elastic case is practically zero. Differences start in the hardening regime. However, these are significantly smaller than in the softening regime. In other words, in the softening regime the macro-level response is extremely sensitive towards meso-level size changes. These results are shown in figure (4). Macro-level mesh dependence is a topic of further study.

4 CONCLUSIONS

In this paper two issues are analysed: the problem of representative volumes and a multiscale modelling technique, both for linear-elastic and softening material behaviour. Following the procedure, based on the statistical analysis of numerical experiments, it has been shown that the representative volume can be found with relatively high accuracy in the case of linear-elasticity. However, in case of softening a representative volume can not be found. Furthermore, a multiscale procedure has been performed. On the basis of the dependence of the macro-level response with respect to meso-level size a conclusion is made about the applicability of the multiscale frame for linear-elastic and softening material behaviour. This conclusion is presented in table (1).

Furthermore, a multiscale procedure has been performed. On the basis of the dependence of the macro-level response with respect to meso-level size a conclusion can be derived for the applicability of the multiscale frame for linear-elastic and softening material behaviour. This conclusion is presented in table (1).

<table>
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<tr>
<th>Table 1: Multiscale overview.</th>
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<tr>
<td>Results</td>
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<td>meso size dependence</td>
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<td>multiscale</td>
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In the linear-elastic case, in which there was no meso-level size dependence found the multiscale frame can be applied and it gives realistic and accurate results. On the contrary for softening material behaviour, one can expect meso-level size dependence, which questions the applicability of the multiscale method.
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6 REFERENCES

