Representative Volume Size as a Macroscopic Length Scale Parameter

I.M. Gitman, H. Askes & L.J. Sluys
Faculty of Civil Engineering and Geosciences, Delft University of Technology, Delft, Netherlands

ABSTRACT: In order to give a micro-mechanical description of material behaviour the analysis of two homogenisation techniques (first-order or local and second-order or nonlocal) is presented in the paper. The macroscopic length scale parameter in the case of nonlocal homogenisation is found in terms of the representative volume element (RVE) size. The dependence of the length scale parameter on the RVE size is investigated for the two schemes, and it is found that the first-order homogenisation scheme behaves more realistic in the sense of convergence of the macroscopic response with increasing RVE size, although a macroscopic length scale is lacking in this scheme.

Keywords: multiscale, first-order homogenisation, second-order homogenisation, RVE, length scale

1 INTRODUCTION

In order to describe and analyse the behaviour of heterogeneous materials different approaches can be used. First of all these approaches can be classified with respect to the scale of interest: one can be interested in a structure as such (so-called macro-scale approach), or one can be more interested in processes which are taking place on the material level (meso-level approach), though sometimes the micro-structure of the material is of big importance (micro-scale approach). When the various scales interact, multiscale analysis gives a better approximation of the real response of the material. The big advantage of the multiscale analysis is that one can take the lower-scale influences into account in order to describe the higher-scale response and vice versa.

In Section 2 the basis of the multiscale procedure is considered: the question of the size of the Representative Volume Element (RVE) is addressed. Section 3 and Section 4 give the detailed analysis of the first and second-order homogenisation techniques.

2 RVE SIZE DETERMINATION

A key ingredient of any multiscale modelling technique is the RVE. This concept is reviewed briefly below.

An important role in multiscale analysis is played by the size of the considered meso-structural or micro-structural unit cell. If this size is, on one hand, large enough to render a statistical homogeneous response, while on the other hand it is small enough compared to the macroscopic structural dimensions, then the meso-structural unit cell is denoted as a Representative Volume Element. The Representative Volume Element (RVE) is widely used in nowadays mechanics (Aidun et al. 1999; Ashihmin and Povyshev 1995; Behrens et al. 1999; Fraldi and Guarracino 2001), etc.

Several methods are available in literature in order to determine the RVE size (Bulsara et al. 1999; Ashihmin and Povyshev 1995). An objective method to determine the size of the RVE was also proposed in (Gitman et al. 2003). The idea of this method is as follows: on the meso-level a three-phase material is assumed (matrix, aggregates and interfacial transition zone). For different aggregate density distributions (fig. 1) a set of realisations is generated, which are then used as input for finite element analyses. Then a statistical analysis, which is based on the Chi-square criterion (1), is used to determine the size of the RVE:
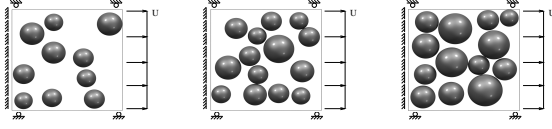
Figure 1: Tension test. Aggregates density distribution a) 30% b) 45% c) 60% in unit cell
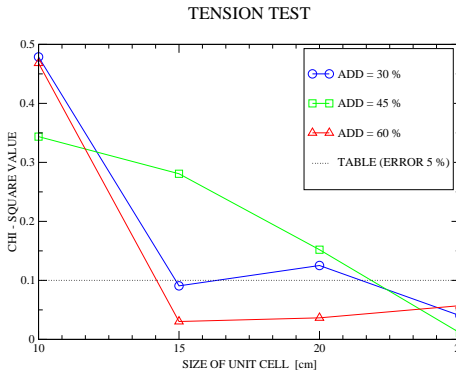

Figure 2: Dependence of Chi-square value on the size of the unit cell

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

where σ_i is the average value of the stress in the current unit cell, $<\sigma>$ is the average value of σ_i in all unit cells (note, that all values of σ are dimensionless), n is the number of unit cells under consideration, i.e. there are n unit cells with the same size but different aggregate distribution. So the idea of the method is to start from the smallest unit cell size, then increase the size of the unit cell and find values of χ^2 using equation (1) until the value of χ^2 is less than the table value of Chi-square coefficient (for a given reliability coefficient and the number of experiments). Then, according to the initially given reliability coefficient and the number of experiments the table value of the Chi-square coefficient can be found. And, as a last step with the help of the curve, fig. 2, (as a crossing of a table value of Chi-square with experimental curve), the corresponding size of the unit cell is determined, which will be considered as a size of RVE for a given value of aggregates density distribution, fig. 3. Thus, for a material with aggregate density distribution 30%, according to the graph, the size of the RVE should be at least 16 cm, for a material with aggregate density distribution 45%, the size of the RVE should be more than 23 cm and for a material with the aggregate den-
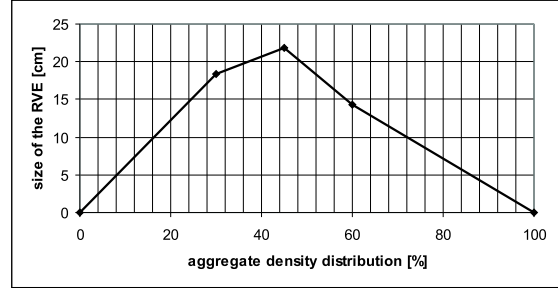

Figure 3: Size of the RVE versus aggregate density distribution

sity distribution equal to 60%, the size of the RVE should not be less than 14 cm. The maximum size of the aggregates was considered as 5 cm. It should be mentioned, that a material with an aggregate density distribution equal to 0% or 100% corresponds to a purely homogeneous material, and in following considerations the size of the RVE of those materials is 0.

3 HOMOGENISATION TECHNIQUES AND THE MACROSCOPIC LENGTH SCALE PARAMETER

Once the size of the RVE has been found, a multiscale procedure can be performed. Below, L denotes the size of the RVE, such that $V_{\rm rve} = L^d$ with d the number of spatial dimensions. The difference between actual and initial configuration is mentioned below as $\bar{V}_{\rm rve}$ and $\mathring{V}_{\rm rve}$, respectively.

There are several steps in the procedure of multiscaling. First of all material is considered on the higher level (macro/structural level). Then in order to improve the accuracy of the response (in the regions of critical activity) the lower level (meso/material level) is analysed. Finally, the results from the meso-level are transfered back to the macro-level. Or in terms of equations: a mechanical loading is applied at macro-level (with a homogeneous structure), this loading should be in equilibrium with the internal forces which are computed from the stresses at meso-level (where the material already has a heterogeneous structure).

The meso-macro connection is used as a constitutive equation on the macro-level. Thus instead of an explicit formulation of the $\sigma - \varepsilon$ relation, data from the meso-level is considered.

Here, according to the scope of the current paper, one more distinction should be made: first-order homogenisation and second-order homogenisation

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techniques. This terminology in a numerical sense was introduced by (Kouznetsova et al. 2002). Below, the terms first-order homogenisation and second-order homogenisation techniques will be used in an analytical context (first-order analytical homogenisation and second-order analytical homogenisation techniques). If we consider the case with only values for stress and strain (in other words in a case of local constitutive equations), then first order homogenisation is used. On the other hand, if we consider also the gradients of these quantities (in case of nonlocal constitutive equations) second order homogenisation may be performed.

These homogenisation techniques are based on averaging. The average value of stresses in the RVE can be computed via

$$< \sigma_{\mathrm{m}} > = \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V \sigma_{\mathrm{m}} dV, \tag{2}$$

in which $\bar{V}_{\mathrm{rve}}$ is the volume of the RVE in the actual configuration.

The average value of the stress at the meso level is equal to the value of the stress at the macro level in the considered integration point:

$$\sigma_{\mathrm{M}} = < \sigma_{\mathrm{m}} >, \tag{3}$$

in which uppercase M corresponds to the macro level and lowercase m to the meso level, respectively.

First of all, according to (2) and (3), values of the stresses on the macro level can be found as

$$\sigma_{\mathrm{M}} = \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V \sigma_{\mathrm{m}} dV = \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V D_{\mathrm{m}} \varepsilon_{\mathrm{m}} dV \tag{4}$$

where D_{m} and ε_{m} are the macroscopic stiffness and strain, respectively. Next, D_{m} and ε_{m} are expanded in Taylor series

$$D_{\mathrm{m}} = D_{\mathrm{M}} + \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} + \mathcal{O}(\delta \mathbf{x}^2) \tag{5}$$

$$\varepsilon_{\mathrm{m}} = \varepsilon_{\mathrm{M}} + \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} + \mathcal{O}(\delta \mathbf{x}^2) \tag{6}$$

Note 1 *Here $\delta \mathbf{x} = \{\delta x_1, ..., \delta x_d\}$ with d the number of spatial dimensions.*

The first-order and the second-order homogenisation schemes are obtained for different truncations of the above series, as is illustrated below.

3.1 *First-order homogenisation*

The first-order homogenisation scheme is obtained when only the first terms in equations (5)-(6) are considered. This yields:

$$D_{\mathrm{m}} = D_{\mathrm{M}} \tag{7}$$

$$\varepsilon_{\mathrm{m}} = \varepsilon_{\mathrm{M}} \tag{8}$$

Then, from (4) it follows that

$$\sigma_{\mathrm{M}} = \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V D_{\mathrm{m}} \varepsilon_{\mathrm{m}} dV = D_{\mathrm{M}} \varepsilon_{\mathrm{M}} \tag{9}$$

It can be concluded now from (9) that in the first-order homogenisation technique there is no length scale parameter on the macroscopic level.

3.2 *Second-order homogenisation*

The second-order homogenisation technique requires the inclusion of also second order terms in the Taylor series when introducing D_{M} and ε_{M} in equations (5)-(6):

$$D_{\mathrm{m}} = D_{\mathrm{M}} + \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \tag{10}$$

$$\varepsilon_{\mathrm{m}} = \varepsilon_{\mathrm{M}} + \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \tag{11}$$

Now the constitutive relation (4) is rewritten in the following form:

$$\sigma_{\mathrm{M}} = \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V D_{\mathrm{m}} \varepsilon_{\mathrm{m}} dV = \tag{12}$$

$$\frac{1}{\bar{V}_{\mathrm{rve}}} \int_V \left(D_{\mathrm{M}} + \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \right) \left(\varepsilon_{\mathrm{M}} + \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \right) dV,$$

or, equivalently, as:

$$\sigma_{\mathrm{M}} = \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V \left(D_{\mathrm{M}} \varepsilon_{\mathrm{M}} + D_{\mathrm{M}} \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} + \right.$$

$$\left. \varepsilon_{\mathrm{M}} \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} + \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \right) dV \tag{13}$$

Note, that D_{M} and ε_{M} are macro values while the integration is carried out on the meso volume. Therefore it is possible to bring D_{M} and ε_{M} outside of the integral and thus:

$$\begin{aligned}
\sigma_{\mathrm{M}} &= \frac{1}{\bar{V}_{\mathrm{rve}}} D_{\mathrm{M}} \varepsilon_{\mathrm{M}} \bar{V}_{\mathrm{rve}} \\
&+ \frac{1}{\bar{V}_{\mathrm{rve}}} D_{\mathrm{M}} \int_V \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV + \\
&+ \frac{1}{\bar{V}_{\mathrm{rve}}} \varepsilon_{\mathrm{M}} \int_V \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV + \\
&+ \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV
\end{aligned} \quad (14)$$

or

$$\begin{aligned}
\sigma_{\mathrm{M}} &= D_{\mathrm{M}} \varepsilon_{\mathrm{M}} + \frac{D_{\mathrm{M}}}{\bar{V}_{\mathrm{rve}}} \int_V \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV \\
&+ \frac{\varepsilon_{\mathrm{M}}}{\bar{V}_{\mathrm{rve}}} \int_V \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV \\
&+ \frac{1}{\bar{V}_{\mathrm{rve}}} \int_V \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV
\end{aligned} \quad (15)$$

The three remaining integrals in (15) are elaborated using integration by parts

- for the first integral:

$$\int_V \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV = \delta \mathbf{x} \varepsilon_{\mathrm{M}}|_{\Gamma} \quad (16)$$

- for the second integral:

$$\int_V \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV = \delta \mathbf{x} D_{\mathrm{M}}|_{\Gamma} \quad (17)$$

- and finally for the third integral:

$$\begin{aligned}
\int_V \frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} \frac{\partial D_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} dV &= \\
\frac{\partial \varepsilon_{\mathrm{M}}}{\partial \mathbf{x}} \delta \mathbf{x} D_{\mathrm{M}} \delta \mathbf{x}|_{\Gamma} &- \\
D_{\mathrm{M}} \nabla_j \nabla_i \varepsilon_{\mathrm{M}} \int_V \delta \mathbf{x} \delta \mathbf{x} dV
\end{aligned} \quad (18)$$

In the case of periodic boundary conditions on the meso level, the values of the integrals (16) and (17) and also the first (boundary) part of (18) are equal to

zero, because then $\delta \mathbf{x}|_{\Gamma} = 0$. As a consequence, (15) can be rewritten as:

$$\sigma_{\mathrm{M}} = D_{\mathrm{M}} \varepsilon_{\mathrm{M}} - \frac{1}{\bar{V}_{\mathrm{rve}}} D_{\mathrm{M}} \nabla_j \nabla_i \varepsilon_{\mathrm{M}} \int_V \delta \mathbf{x} \delta \mathbf{x} dV. \quad (19)$$

Finally the last integral in (19) can be rewritten via

$$\int_V \delta \mathbf{x} \delta \mathbf{x} dV = \int_{\mathring{V}} \frac{1}{J} \delta \mathbf{x} \delta \mathbf{x} d\mathring{V}, \quad (20)$$

where $\mathring{V}$ refers to the initial configuration, and J is the Jacobian transformation

$$J = \frac{\bar{L}_{\mathrm{rve}}^d}{\mathring{L}_{\mathrm{rve}}^d}.$$

Note, that $\bar{V}_{\mathrm{rve}}$ and $\mathring{V}_{\mathrm{rve}}$ are representative volumes in the actual and initial configurations, respectively, and $\bar{L}_{\mathrm{rve}}^d$ and $\mathring{L}_{\mathrm{rve}}^d$ are the corresponding sizes of the RVE.

With $\delta \mathbf{x} = \{\delta x_1, ..., \delta x_d\}$ it is written that

$$\int_{\mathring{V}} \frac{1}{J} \delta \mathbf{x} \delta \mathbf{x} dV = \int_{\mathring{V}} \frac{1}{J} \delta x_i \delta x_j d\mathring{V}. \quad (21)$$

If we take the above integral we can consider two situations:

1. $i = j$: carrying out the integration, one obtains

$$\int_{\mathring{V}} \frac{1}{J} \delta x_i \delta x_i d\mathring{V} = \frac{1}{12} \frac{\mathring{L}_{\mathrm{rve}}^{2d+2}}{\bar{L}_{\mathrm{rve}}^d}. \quad (22)$$

2. $i \neq j$: in this case the integral vanishes:

$$\int_{\mathring{V}} \frac{1}{J} \delta x_i \delta x_j d\mathring{V} = 0. \quad (23)$$

Because of the results in (22) and (23) only same index derivatives are considered in (19) which yields

$$\nabla_j \nabla_i \varepsilon_{\mathrm{M}} \rightarrow \nabla_i \nabla_i \varepsilon_{\mathrm{M}} \rightarrow \nabla^2 \varepsilon_{\mathrm{M}}. \quad (24)$$

As a consequence (19) can be rewritten as

$$\sigma_{\mathrm{M}} = D_{\mathrm{M}} \varepsilon_{\mathrm{M}} - \frac{D_{\mathrm{M}}}{12} \frac{\mathring{L}_{\mathrm{rve}}^{2d+2}}{\bar{L}_{\mathrm{rve}}^{2d}} \nabla^2 \varepsilon_{\mathrm{M}} \quad (25)$$

Note, that (25) only contains macroscopic parameters plus a coefficient that precedes the ∇^2-operator. This coefficient has the dimension of length squared and thus acts as a macroscopic length scale parameter.

Note 2 *In case of small deformations the macroscopic length scale parameter can be rewritten simply as* $\frac{1}{12}L_{rve}^2$.

3.3 *Aifantis' gradient elasticity model*

Equation (25) bears close similarities with the gradient elasticity model proposed by Aifantis and coworkers (Ru and Aifantis 1993; Altan and Aifantis 1997):

$$\sigma_M = D_M(\varepsilon_M - l^2\nabla^2\varepsilon_M) \tag{26}$$

where l is a macroscopic length scale parameter. According to (25) and (26), the phenomenological parameter l can be connected with the size of the RVE via:

$$l^2 = \frac{1}{12}\frac{\mathring{L}_{\text{rve}}^{2d+2}}{\bar{L}_{\text{rve}}^{2d}}. \tag{27}$$

4 DEPENDENCE ON THE RVE SIZE

Following the concept of the RVE, it is known, that with increasing size, structural behaviour should not be affected. In other words, it should be verified whether the macroscopic response converges with increasing RVE size.

4.1 *First-order homogenisation*

As a representative example of the first-order homogenisation technique, the tension test is considered. The response of the linear elastic material is analysed in terms of the reaction forces on the macro-level for a given imposed displacement. Schematically, the procedure is presented in fig.4. The unit cell on the meso-level is composed of aggregates, matrix material and an interfacial transition zone.

Following the procedure of the RVE size determination, for the material with the aggregates density distribution equal to 30% the size of the RVE should be at least 16cm (fig.1). In order to analyse the dependence on the RVE, the sizes 10cm and 25cm were taken. Next, the statistical analysis of the reaction forces on the macro level shows that the sample standard deviation (Jaynes 1995) in the case of the size of the unit cell equal to 10cm is $S = 6.65$ and
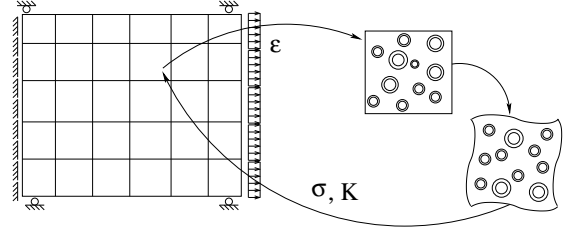

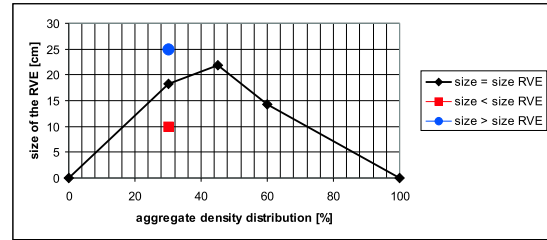Figure 4: Multiscale test. First-order homogenisation

Figure 5: Different sizes of the the meso-level unit cells

$S = 0.37$ in case of the size of the unit cell equal to 25cm. Thus, the sample standard deviation in the first case ($V < V_{\text{rve}}$) is much larger than in the second case ($V > V_{\text{rve}}$). In other words, with increasing size of the unit cell on the meso level the deviation of the macroscopic response approaches zero, i.e. the macro response converges.

4.2 *Second-order homogenisation*

Using the analogy with the first order homogenisation scheme, the dependence on the meso-level RVE size of the macro response can be analysed also for the second order analytical homogenisation technique.

Unlike the first-order homogenisation scheme, here the size of the RVE is linearly connected to the macroscopic length scale parameter (as it was shown in (27)), which plays a crucial role in the definition of the macroscopic response (25). Thus, increasing the RVE size does not lead to convergent macroscopic behaviour.

Numerical homogenisation (Kouznetsova et al. 2002) seems to confirm these analytical findings.

5 CONCLUSIONS

The homogenisation schemes have been compared in terms of (i) the appearance of a macroscopic length scale, and (ii) the dependence of the macroscopic response on the RVE size. If first-order ho-

mogenisation is chosen to be used in a multiscale analysis, no macroscopic length scale parameter is introduced, which is acceptable in applications such as linear-elasticity and hardening processes, but causes problems in softening applications (where a length scale parameter needs to be included in order to maintain well-posedness of the problem). In the last case the second-order homogenisation technique seems to work better on one hand: a macroscopic length scale parameter is found which is related to the size of the RVE. But on the other hand a big disadvantage of the second-order homogenisation technique is its limited applicability: from the analytical derivation it became clear that the macroscopic length scale depends *linearly* on the RVE size, so that the macroscopic response does not converge with increasing RVE size. In contrast, the first-order homogenisation procedure does not depend on the size of the RVE — increasing the RVE size leads to a convergent macroscopic response (as long as an RVE exists).

Thus, for cases of linear elasticity and hardening applications (where an RVE exists) the first-order homogenisation technique gives better (more realistic) results. Schematically, all the above can be placed in a table:

Results		macro length scale param.	convergence in macro response
Analytic.	I	no	yes
	II	yes	no
Numeric.	I	no	yes
	II	yes*	no*

where I and II correspond to the first and second order homogenisation techniques, respectively.

In this paper analytical results for first- and second order homogenisation have been presented. Numerical first-order homogenisation was used for a linear elastic problem to prove the convergence of the macroscopic response with respect to RVE size. Numerical first- and second-order homogenisation was studied by Kouznetsova (Kouznetsova et al. 2002) for hardening materials (these results are marked with an asterisk in the table).

For softening applications (where a macroscopic length scale parameter is required), the second-order homogenisation technique seems to provide better results: a macroscopic length scale parameter is found (both analytically and numerically). But intuitive preference to use a second-order homogeni-

sation technique while considering softening processes can also be questioned: problems arise when finding the size of the RVE, one could argue that it even does not exist (Lacy et al. 1999; Graham and Yang 2003). Taking the last issue as working hypothesis, then neither first nor second-order homogenisation technique can be implemented in softening applications.

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