MULTI-SCALE MODELING OF SOFTENING MATERIALS

O. Lloberas, A.Simone and L.J. Sluys

Faculty of Civil Engineering and Geosciences, Delft University of Technology, The Netherlands

Abstract

This paper presents an assessment of a two-scale framework for the study of softening materials. The procedure is based on a hierarchical Finite Element (FE) scheme in which computations are performed both at macro and mesoscopic scale levels. The methodology is chosen specifically to remain valid when the scales are coupled which is frequently encountered in fracture processes of heterogeneous materials.

The effect of the boundary conditions chosen to construct the meso-scale problem is studied in this contribution by comparing multiscale and monoscale analysis of an equivalent problem. It is shown in this study that macroscopic mesh size dependence is encountered when using linear interpolated boundary displacements at the interface between meso-specimens.

An improvement to the linear interpolated boundary displacements is presented which proves to be more adequate when strain localisation phenomena is encountered at the interface of the meso-specimens. The specific upscaling procedure for the improved boundary conditions remains an issue of ongoing research.

1. INTRODUCTION

The increasing performance of modern computational tools has stimulated to model many engineering materials at a significant detailed level. This is the case for multiscale strategies which aim to simulate the processes which originate at a lower material scale such as localisation and fracture.

Different approaches can be found in literature which aim at obtaining a more accurate response of the material via the computations at a lower scale level. During the recent years approaches have been developed to include the classical homogenisation theories in to a nested computational framework. This is the case of computational homogenisation techniques (see i.e. [1] and [2]) where the link between the upper and lower scale is established at the macroscopic integration point of the structural specimen. The constitutive information at the macroscopic Gauss point is given by the solution of a mesoscopic boundary value problem over a representative volume (RVE) of the material. Non-linear phenomena is naturally captured due to the incremental iterative formulation of the scheme in which a numerical technique (i.e. Finite Element method) is needed to solve both upper and lower-scale problems.

The key ingredient of these techniques is the assumption made to downscale the information and build the boundary value problem at the lower level. Different assumptions are explained in [3] which have an influence on the resulting constitutive law used at the upper level. As shown in [4], difficulties are found in order to determine the size of the representative volume when the material shows softening and localisation phenomena. It can be proved that when combining this technique with a constitutive model that allows for softening and localisation, both macro-element and meso-level size dependence are found [4].

The former fact is linked to a lack of regularisation upon mesh refinement whilst the latter is a purely phenomenological issue related to the non existence of an RVE for the softening regimes.

An attempt to overcome the latter drawbacks is to formulate a scheme in which upper and lower scales remain coupled. This is the case of *strong coupling multiscale techniques* as described in [5] and [6] by Ibragimbehovic and Markovic. The idea is to assign a meso-specimen to each macro-element and perform the data exchange at the macroscopic element level instead of the Gauss point level. The scales are coupled via localised Lagrangian multipliers which provide compatibility for meso and macro displacement fields. This technique is taken in this study for the case of a *displacement interface* and assessed for softening materials. In the case where the displacements at the interface are forced to be compatible without any extra constraint the technique can be compared to *substructuring* or *domain decomposition techniques* (i.e. [7]) where the different domains of study would be represented by the macroscopic elements themselves.

Other techniques (see [8] and [9]) are based on the superposition of a global (upper level) and a local (lower level) solution field over a certain domain. The upscaling is performed this time enriching the global shape functions via the solution field of the local problem. The enrichment at the boundaries of the local problem needs to be zero and, for this reason, the local domain should always explicitly contain all non-linearities and complex phenomena (i.e. cracking and strain localisation) that can not be described uniquely at the global domain.

In the following a formulation is presented for the *strong coupling multiscale technique* with a *displacement interface*.

2. METHODOLOGY

In this section the formulation of the strong coupling multiscale framework is introduced for the case of a displacement interface based on linear interpolation of the macroscopic displacement field along the mesoscopic boundaries and an improved displacement interface based on the geometrical compatibility between upper and lower scales.

2.1 Framework formulation

In order to couple the scales every macro element is assigned a corresponding meso-cell with identical shape and dimensions. Macro-elements are constituted in this study by four nodded bilinear elements and meso-specimens are formed, at the same time, by an arbitrary FE type. At the macro level no constitutive law is specified whereas at the meso-level all phases of the heterogeneous material are identified by its inelastic law. The data exchange between upper and lower levels is performed at the element level of the macro computations (see Figure 1) where element quantities are formed after the solution of the corresponding meso boundary value problems. An advantage of such a scheme is that all mesoscopic computations can be performed in parallel.

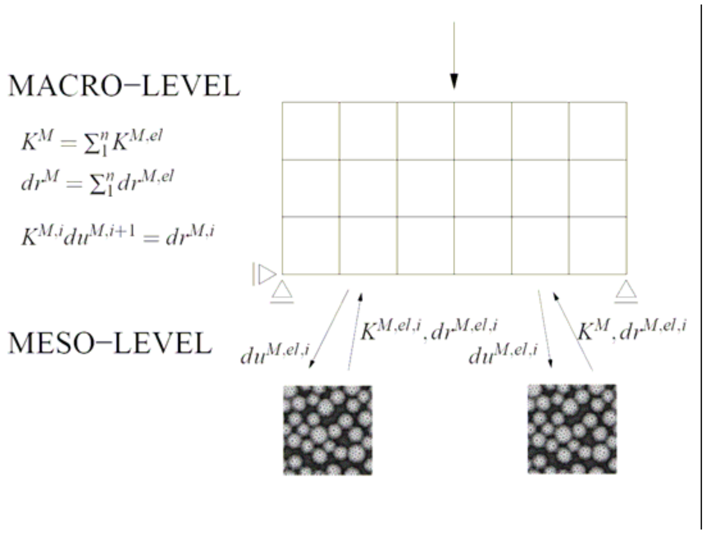

Figure 1: Framework scheme

At each macro iteration (i) the linearised system of equations

$$\mathbf{K}^{M,i} d\mathbf{u}^{M,i+1} = d\mathbf{r}^{M,i} \qquad (1)$$

needs to be solved, where here the superscripts M and m are used to indicate macro and mesoscopic quantities respectively. Each macro element is assigned a meso specimen for which a boundary value problem can be constructed based on the iterative displacements of the four corner nodes. The downscaling strategy is summarized in Eq. (2).

$$\mathbf{u}^{m,el,i} = \mathbf{T}^{el}\mathbf{u}^{M,el,i}, \qquad (2)$$

where the transformation matrix $\boldsymbol{T}$ is introduced which sets the relation between the displacement of the corner nodes of each macro element and the corresponding displacements along the boundaries of the mesoscopic cell.

The corresponding linearised problem to be solved at the meso-level for each iteration (j) reads

$$\mathbf{K}^{m,j} d\mathbf{u}^{m,j+1} = d\mathbf{r}^{m,j}\,. \qquad (3)$$

After reaching equilibrium at the meso-level the upscaling of the quantities is performed in two steps as illustrated in Eqs. (4) and (5). First the static condensation of Wilson [10] is employed to project the information to the boundaries of the meso-specimen

$$\hat{\mathbf{K}}^{m,el} = \mathbf{K}_{pp}^{m,el} - \mathbf{K}_{pf}^{m,el}(\mathbf{K}_{ff}^{m,el})^{-1}\mathbf{K}_{fp}^{m,el} \qquad (4)$$

$$d\hat{\mathbf{r}}^{m,el} = d\mathbf{r}_{p}^{m,el} - \mathbf{K}_{pf}^{m,el}(\mathbf{K}_{ff}^{m,el})^{-1} d\mathbf{r}_{f}^{m,el}\,,$$

obtaining the condensed stiffness matrix and residual vector respectively. Second this information is transformed using the transformation matrix $\boldsymbol{T}$ into macroscopic quantities to be used in Eq. (1) for each macro iteration.

$$\mathbf{K}^{M,el,i} = (\mathbf{T}^{el})^{T}\hat{\mathbf{K}}^{m,el}\mathbf{T}^{el} \qquad (5)$$

$$d\mathbf{r}^{M,el,i} = (\mathbf{T}^{el})^{T} d\hat{\mathbf{r}}^{m,el}\,.$$

2.2 Displacement interface

The simplest choice of the displacement interface is the linear interpolation of the displacements at the corners of the macroscopic specimen. In this case it is trivial to construct ***T*** such it accomplishes Eq. (2). Figure 2 (left) illustrates the linear interpolated interface for a quadrilateral macro element which has a corresponding cell meshed with nine regular quadrilateral elements.

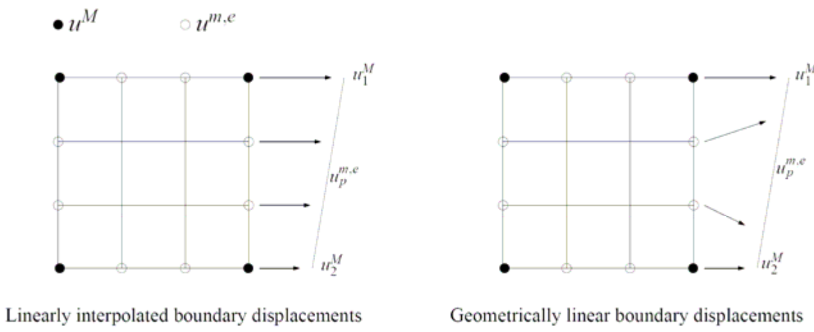

Figure 2: Displacement interfaces

An alternative displacement interface is to preserve the macrosopic deformed configuration allowing the mid boundary nodes of the meso cell to move freely along the deformed edge. The geometrically linear boundary displacements (Figure 2 (right)) can be seen as a weak constraint that would allow more flexibility to the interface.

In this strategy the downscaling is accomplished by imposing the displacement at the four corner nodes in an exact way and setting a multifreedom constraint to the mid boundary nodes of the meso cell. This multifreedom constraint can be imposed using Lagrange multipliers, the penalty method or the master slave method. The weak constraint sets, in this case, the slope to each mid boundary node according to the deformed configuration dictated by the macroscopic corner nodes. Figure 3 shows schematically the deformed configuration of a side of the quadrilateral. The linear deformed configuration can be formulated as a multifreedom constrain using the penalty method by means of the penalty element stiffness equation shown in Eq. (6).

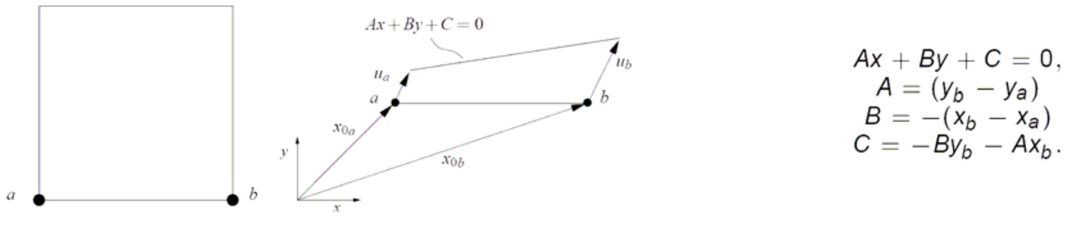

Figure 3: Multifreedom constraint formulation

$$\varpi \begin{bmatrix} AA & AB \\ BA & BB \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = -\omega \begin{bmatrix} AC \\ BC \end{bmatrix}. \tag{6}$$

The scalar ω denotes the penalty weight used to enforce the constraint. Eq. (6) can be rewritten in terms of the displacement field increment and assembled to the mesoscopic stiffness at the corresponding positions of the boundary degrees of freedom.

3. RESULTS

In this section two examples are presented in which the multiscale framework is assessed for softening materials. The third example shows the performance of the geometrically linear boundary displacements when an arbitrary orientation for the strain localisation is encountered. All computations are performed in 2D assuming plain strain. The model used at the meso-level is a *gradient enhanced damage model* (see [11]) where an exponential damage evolution law and a Mazar's definition of the non-local equivalent strain are considered.

3.1 Macroscopic mesh size sensitivity

In this example a tension test is performed to a quadrilateral sample containing four voids aligned vertically in its left edge as depicted in Figure 4a (upper left). The test consists on pulling from the right edge of the specimen until the load carrying capacity is reached and the cell starts softening localising the strains around the aligned voids. A single-scale analysis is performed meshing the structure depicted in Figure 4a (upper left) using three-nodded triangular elements. The same test is simulated now using the multiscale framework with a 1x1, 2x2 and a 3x3 macro element discretisation (Figure 4a (upper right, lower left and lower right)). Each of the macro elements have a corresponding meso-cell meshed using three nodded triangular elements and containing the voids as shown in the upper left part of Figure 4a.

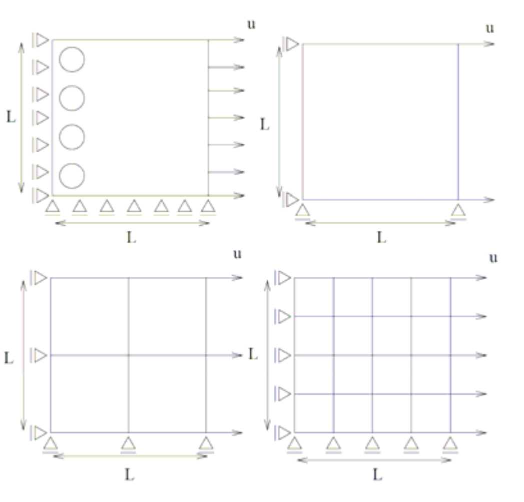

Figure 4a: Multiscale discretisation

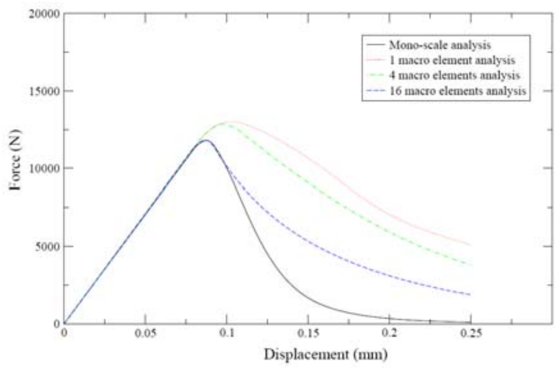

Figure 4b: Mechanical response

The force versus displacement graphic at the right boundary is depicted in Figure 4b. It is observed that the dissipated energy is different for the monoscale and the multiscale analysis with 1x1, 2x2 and 3x3 macro elements. The coarser the macroscopic discretisation the more ductile the behaviour which is, at the same time, drifting away from the true monoscale response. This effect is explained considering that the linear interpolated boundary displacements do not allow the strains to localise along the boundary. For this reason the area that is experiencing unloading during the softening regime is lower than in the monoscale analysis causing a more ductile overall behaviour.

3.2 Displacement interface test

A tensile test is imposed to a quadrilateral sample containing three voids in its center as shown in Figure 5a (upper right). The specimen is tested by means of a single scale analysis, a multiscale analysis (using linear interpolated boundary displacements) and using the geometrically linear boundary displacements applied to a single macroscopic element (1x1 macro-discretisation). The mechanical response at the right boundary of the cell is shown in Figure 5b.

It can be observed that the dissipated energy between the single scale analysis and its equivalent test using the geometrically linear boundary displacements is practically the same. Nevertheless, when comparing these two graphics with the one obtained using the former displacement interface the behaviour is slightly stiffer during the elastic regime and more ductile along the softening regime.

The geometrically linear boundary displacements allow for localisation to take place at the boundary in a natural way. For this reason the overall behaviour is much more similar to the one observed at the single scale test. Hence the area where strain is localizing is comparable and this is translated to the overall response.

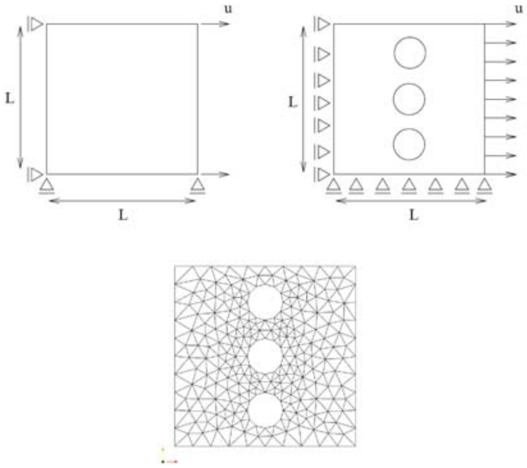

Figure 5a : Loading test

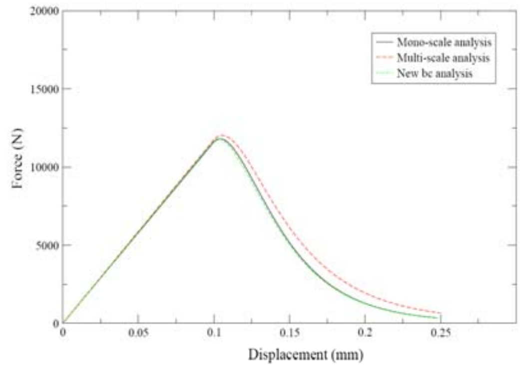

Figure 5b : Mechanical response

3.3 Localisation test

In this section the later displacement interface is used with a specimen containing three voids aligned diagonally as depicted in Figure 6. The specimen is pulled from opposite corners. Displacement, local equivalent strain and damage contours are shown in Figure 7. The deformed geometry of the edges is linear as dictated by the constraint type. Nevertheless localisation can naturally take place at the boundaries and corners of the specimen. The displacement interface is compatible with an arbitrary orientation of the strain localisation.

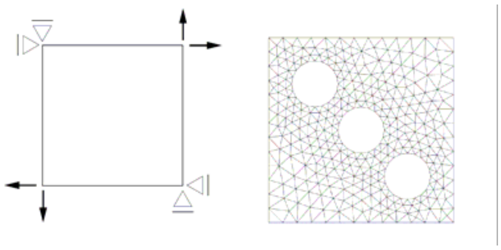

Figure 6: Loading test

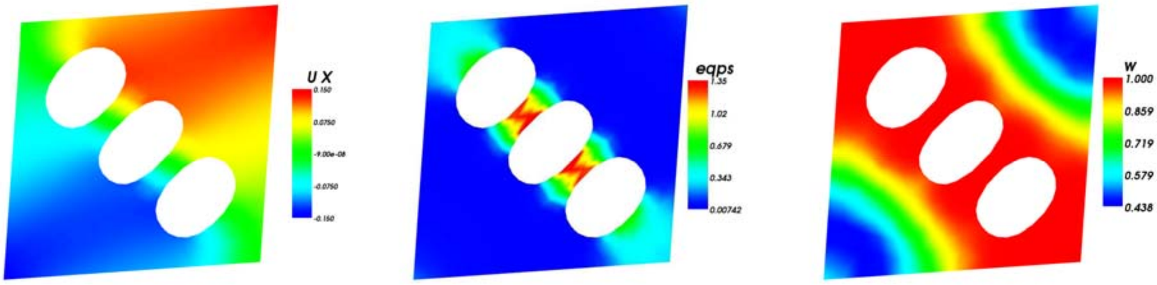

Figure 7: Field contours of the deformed specimen

4. CONCLUSIONS

A strong coupling multiscale framework is assessed in this study for materials that show softening and localisation. The choice of a displacement interface based on a linear interpolated boundary displacements does not seem to be adequate for this type of problems. Macroscopic mesh size dependency is observed. The overall response of the specimen is more ductile when the macro structure is discretised with a coarser mesh.

When the displacement interface is set using geometrically linear boundary displacements, localisation can take place naturally at the boundaries during the softening regime. The energy dissipation is comparable to the single scale analysis, hence seems a more adequate choice to tackle these kind of problems.

A transformation matrix is not trivial to find for this kind of displacement interface and the downscaling is performed using multi freedom constraints at the mid boundary nodes. For this reason the upscaling technique needs to be tailored for this particular case and it is an issue of ongoing research.

REFERENCES

[1] Feyel, F., 'A Multilevel finite element method (fe^2) to describe the response of highly non-linear structures using generalised continua', *Comp. Methods Appl. Mech. Engrg.* **192** (2003) 3233-3244.

[2] Geers, M.G.D., Kouznetsova, V.G. and Brekelmans, W.A.M., 'Multi-scale first-order and second-order computational homogenization of microstructures towards continua', *Int. J. Multiscale Comput. Engrg.* **1** (2003) 371-386.

[3] Miehe, C. and Koch, A., 'Computational micro-to-macro transitions for discretized micro-structures undergoing small strain', *Archives in Applied Mechanics.* **72** (2002) 300-317.

[4] Gitman, I.M , 'Representative volumes and multiscale modelling of quasi-brittle materials', PhD thesis (Technishe Universiteit, Delft, 2006).

[5] Marcovic, D. and Ibrahimbegovic, A., 'On micro-macro interface conditions form microscale based FEM for inelastic behaviour of heterogeneous materials', *Comp. Methods Appl. Mech. Engrg.* **193** (2003) 5503-5523.
[6] Marcovic, D. and Ibrahimbegovic, A., 'Strong coupling methods in multi-phase and multi-scale modelling of inelastic behaviour of heterogeneous structures', *Comp. Methods Appl. Mech. Engrg.* **192** (2003) 3089-3107.
[7] Przemieniecki, J.S., 'Theory of matrix structural analysis', McGraw-Hill (USA, 1968).
[8] Duarte, C.A. and Kim, D.-J., 'Analysis and Applications of a Generalized Finite Element Method with Global-Local Enriched Functions', *Comp. Methods Appl. Mech. Engrg.* (2006) (TO BE COMPLETED).
[9] Duster, A., Niggl, A. and Rank, E., 'Applying the hp-d method of the FEM to locally enhance dimensionally reduced models', *Comp. Methods Appl. Mech. Engrg.* **196** (2007) 3524-3533.
[10] Wilson, E.L., 'The static condensation algorithm', *International Journal for Numerical Methods in Engineering.* **8** (1974) 198-203.
[11] Peerlings, R., 'Enhanced damage modelling for fracture and fatigue', PhD thesis (Eindhoven University of Technology, Eindhoven, 1999).