Non-linear Computational Homogenization Experiments

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Abstract: Numerical homogenization is based on the usage of finite elements for the description of average properties of materials with heterogeneous microstructure. The practical steps of the method and representative examples related to masonry structures are presented in this paper. The non-linear Representative Volume Element (RVE) of the masonry is created and solved within COMSOL Multiphysics. Parametric analysis has been chosen and used for the description of the loading. Thus, several RVE models with gradually increasing loading are solved. Results concerning the average stress and strain in the RVE domain are then calculated, by using the subdomain integration of COMSOL. In addition, the tangent stiffness is estimated for each loading path and loading level. Finally, two databases for the tangent stiffness and the stress are created, metamodels based on MATLAB interpolation are used, and an overall non-linear homogenization procedure of masonry macroscopic structures, in a FEM^2 approach, is considered. Results are compared with direct heterogeneous macro models.
Keywords: Homogenization, Multi-scale, Masonry, FEM^2

1. Introduction

Computational homogenization is used for the investigation of the structural behaviour of complex, heterogeneous structures, by considering a representative microscopic sample of the material, and then projecting the average material characteristics in the macroscopic, structural scale. Other methods, which are applied directly in the macroscopic scale, can also be found in the literature [1, 2].

Several materials, like masonry and composites can be simulated by using computational homogenization. In this article, a method describing the study of masonry using COMSOL Multiphysics, is presented.

Several different homogenization approaches have been proposed in the literature. Among them analytical and numerical techniques are included. Analytical methods can be more accurate in the description of the micro structure [3] but are usually applicable in simpler models. On the other hand, numerical methods may be used for the simulation of complex patterns of micro models, over a statistically defined representative amount of material [4].

Numerical/computational homogenization can be extended to cover several non-linear effects, like contact, debonding, damage and plasticity [5]. According to numerical homogenization, a unit cell is explicitly solved and the results are then used for the determination of the parameters of a macroscopic constitutive law [6]. From another point of view, multi-level computational homogenization incorporates a concurrent analysis of both the macro and the microstructure, in a nested multi-scale approach [7-10]. Within this method, the macroscopic constitutive behaviour is determined during simulation, after solving the microscopic problem and transferring the information on the macroscopic scale. This approach, which is generally called FEM^2, offers the flexibility of simulating complex microstructural patterns, with every kind of non-linearity.

In the present work, a computational homogenization approach is presented, for the study of non-linear masonry structures. COMSOL Multiphysics parametric analysis is used for the simulation of a non-linear masonry Representative Volume Element (RVE), under several loading paths. In each loading path, linear displacement boundary conditions are incrementally applied in the boundaries of the RVE. After solution of the microscopic structure, the average stress is calculated within COMSOL. As a result, a strain-stress database is created. In addition, for each loading path and each loading level, three test incremental loadings are applied to the RVE. Consequently, tangent stiffness information is obtained for each particular loading path and loading level and a second strain-stiffness database is obtained. Based on these databases, and MATLAB-based interpolation for the creation of a metamodel, a computational homogenization model, in a FEM^2 sense, is created for the macroscopic analysis of masonry structures. Comparison with direct heterogeneous macroscopic models shows that the adopted procedure leads to satisfactory results.

2. Computational homogenization: a short introduction

Computational homogenization is used for the simulation of complex, non-linear structures of composite, heterogeneous materials. The approach adopted in this article is related to the concurrent analysis of the macroscopic and the microscopic structure. According to the classical formulation of the method, two nested boundary value problems are concurrently solved. The initial heterogeneous macroscopic structure is equivalent with a homogeneous one, in each Gauss point of which, an RVE is corresponding. This RVE includes every heterogeneity and non-linearity of the material.

According to the Hill-Mandel condition or energy averaging theorem, the macroscopic volume average of the variation of work equals to the local work variation, on the RVE [11]:

$$\boldsymbol{\sigma}^M : \boldsymbol{\epsilon}^M = \frac{1}{V_m}\int_{V_m} \boldsymbol{\sigma}^m : \boldsymbol{\epsilon}^m dV_m \tag{1}$$

Three type of loading states, which satisfy the above condition, can be applied to the RVE: a) prescribed linear displacements, b) prescribed tractions, c) periodic boundary conditions.

In particular, according to the Hill-Mandel principle a macroscopic strain is the loading of the RVE through linear or periodic boundary conditions. After analysis and convergence of each RVE in every Gauss point, results concerning the average stress and the consistent stiffness are given back to the macroscopic structure, Figure 1. This way, the macroscopic constitutive behaviour is numerically obtained. Thus, no assumption for the constitutive law of the macroscopic structure is initially required.

A significant step of the overall procedure is related to the estimation of the average quantities of the microscopic stress and strain. Generally, they are given by the averaging relations (2).

In the next paragraphs the way that these quantities are estimated within COMSOL, is presented.

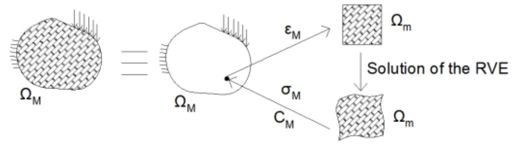


Figure 1. Schematic representation of the concurrent multi-scale homogenization

$$<\boldsymbol{\epsilon}>_{V_m} = \frac{1}{V_m}\int_{V_m} \boldsymbol{\epsilon}^m dV_m, \quad <\boldsymbol{\sigma}>_{V_m} = \frac{1}{V_m}\int_{V_m} \boldsymbol{\sigma}^m dV_m \tag{2}$$

3. Use of COMSOL Multiphysics

3.1 Brief description of the proposed concept

The key idea of the present work is to replace the microscopic simulation of the RVE, which is considered within each time step of the computational homogenization method, with two databases containing information related to the stress and the stiffness of the macro model. This information is transferred back to the macroscopic structure.

Thus, instead of solving the RVE in each Gauss point and time step, which is a time consuming procedure, an interpolation of the proper quantity from the databases is considered. This concept has the following steps:

a) Creation of a masonry RVE with COMSOL Multiphysics. It consists of the bricks and the mortar joints, thus the material that connects the bricks. The non-linearity of this model is concentrated on the mortar joints by using a perfect plasticity law. The brick parts are linear.

b) A number of loading paths are developed and applied to the RVE. To do this, plane stress parametric analysis from the structural mechanics module is used. Each loading path consists of a number of increments.

Linear boundary conditions are applied as loading to the boundaries of the RVE. The “Prescribed displacement” option is chosen in the boundary settings.

c) After analysis of each RVE is completed, the average stress is calculated, within COMSOL.

d) Steps b) and c) are repeated for each loading path and each loading level, but now three test incremental loadings are applied to the RVE. Then, by incrementally solving the Hooke’s law, tangent stiffness information is obtained for the particular loading path and level.

e) Two databases have been created: one that corresponds strains to stresses and another that corresponds strains to stiffness information. These are incorporated in a FEM^2 computational homogenization scheme developed with MATLAB, for the simulation of macroscopic masonry structures.

f) Comparison of the results with direct heterogeneous macroscopic models created in other commercial software packages is used to evaluate the whole procedure.

3.2 Detailed description of the proposed concept

A crucial role for the successful implementation of the present concept plays the accurate creation of the databases. COMSOL capability of parametric analysis offers the opportunity of creating a big number of models, fast and easy.

The linear displacement loading is generally given by relation:

$$\mathbf{u}|_{\partial V_m} = \boldsymbol{\epsilon}^M \mathbf{x} \quad (3)$$

where a loading strain $\boldsymbol{\varepsilon}^M = [e_{xx} \; e_{yy} \; e_{xy}]^T$ is applied to the boundaries ∂V_m of the RVE. With $\mathbf{x}$ is denoted the matrix with the undeformed coordinates of the boundary nodes. Relation (3) is rewritten [12], for each boundary node of the RVE:

$$u_x = (e_{xx})x + (0.5e_{xy})y \quad (4a)$$

$$u_y = (e_{yy})y + (0.5e_{xy})x \quad (4b)$$

In order to simulate every possible combination between e_{xx}, e_{yy} and e_{xy} in three dimensional space, only one parameter can be used in COMSOL. To do this, two angles (a, b) between these quantities are introduced, according to Figure 2.

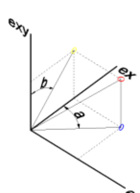


Figure 2. Three dimensional scanning of the "strain space"

Consequently, one parameter ("param") is incorporated in relations (4), within the "Prescribed displacement" option of the boundary settings. In the parameter both positive, and negative values are given, namely for the considered example: 0.1:12:2940.1 and -2940.1:12:-0.1. This parameter, together with angles a and b, substitute e_{xx}, e_{yy}, e_{xy} of relations (4), leading to equations (5). These are the final equations that are used in COMSOL (where *k1*, *k2*, *k3* are only some additional numbers used to correct the displacements, according to the desired limits).

$$R_x = u_x = (cos(b)sin(a)(k1param))x + (sin(b)(0.5k3param))y \quad (5a)$$

$$R_y = u_y = (cos(b)cos(a)(k2param))y + (sin(b)(0.5k3param))x \quad (5b)$$

It is then possible to obtain a satisfactory number of combinations between members of the strain vector $\boldsymbol{\varepsilon}^M$, proportional to the different combinations of the (a, b) angles. In particular, 7x13=91 different angle (a, b) combinations have been test, with COMSOL (angles in degrees):

(a, b) = (a, 90), (a, 60), (a, 30), (a, 0), (a, -30), (a, -60), (a, -90), for a=0:30:360.

COMSOL script files were created for the fast completion of these analyses. Within each script, the 7 combinations (a, 90) until (a, -90), for a=0:30:360, were considered. Each analysis was conducted from COMSOL script, run m-file capability.

The whole numerical scheme were repeated twice: first for deriving the average macroscopic stress, thus the creation of the strain-stress database, second for obtaining the stiffness of the macro model, thus the strain-stiffness database.

To obtain the average macroscopic stress for each time step and load path, the subdomain integration, postprocessing capability of COMSOL, was used. With this tool were selected as predefined quantities the "sx normal stress global sys.", "sy normal stress global sys." and "sxy shear stress global sys.", while as subdomain selection the whole domain of the RVE was chosen. Commands containing this information were added in the end of each COMSOL script file. Then the averaging relation (2) for the stresses was written.

The average strain of each analysis was obtained similarly, by incorporating in the COMSOL script "ex normal strain global sys.", "ey normal strain global sys." and "exy shear strain global sys." and the average relation of equations (2), for the strains. However, it is noted that according to homogenization theory, the average strain is a priori a known quantity, as it is equal to the loading strain.

Finally a MATLAB .mat file was asked, where the averages strains and stresses were incorporated. This file is used in the next step of the proposed method.

The procedure was repeated for deriving the stiffness information of the macroscopic model. For this reason, for every load path and load (strain) level, three test increments of the strain were considered, and three average incremental stresses were calculated, respectively. Then, the elasticity tensor, which is the stiffness information for the macroscopic model, was calculated by using Hooke's law, according to equations (6).

$$[\delta\boldsymbol{\epsilon}^M] = [\delta\boldsymbol{\epsilon}_1^M \quad \delta\boldsymbol{\epsilon}_2^M \quad \delta\boldsymbol{\epsilon}_3^M] \tag{6a}$$

$$[\delta\boldsymbol{\sigma}^M] = [\delta\boldsymbol{\sigma}_1^M \quad \delta\boldsymbol{\sigma}_2^M \quad \delta\boldsymbol{\sigma}_3^M] \tag{6b}$$

$$[\delta\boldsymbol{\sigma}^M] = \mathbf{C}^M[\delta\boldsymbol{\epsilon}^M] \Rightarrow \mathbf{C}^M = [\delta\boldsymbol{\sigma}^M][\delta\boldsymbol{\epsilon}^M]^{-1} \tag{6c}$$

In plane stress elasticity, the elasticity tensor $\boldsymbol{C}^M$ is a 3x3 tensor, while each of the $\delta\boldsymbol{\varepsilon}_1{}^M$, $\delta\boldsymbol{\varepsilon}_2{}^M$, $\delta\boldsymbol{\varepsilon}_3{}^M$, $\delta\boldsymbol{\sigma}_1{}^M$, $\delta\boldsymbol{\sigma}_2{}^M$, $\delta\boldsymbol{\sigma}_3{}^M$ is 3x1 tensor; thus the $[\delta\boldsymbol{\varepsilon}^M]$, $[\delta\boldsymbol{\sigma}^M]$ are 3x3 tensors, respectively.

After the whole analysis scheme with COMSOL was completed, the resulted data was incorporated in a FEM^2 computational homogenization model for the study of masonry structures, according to the following sections.

3.3 The RVE finite element model in COMSOL

Before the presentation of the overall homogenization procedure, some details of the finite element model for the RVE created within COMSOL are given. The geometry of the RVE is shown in Figure 3.

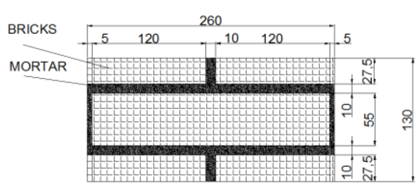


Figure 3. Geometry of the masonry RVE (dimensions in mm)

Rectangular plane stress elements have been used for the simulation of the model, Figure 4. The out of plane thickness of the structure is taken equal to 70mm. For both the brick and the mortar, isotropic elasticity is considered. Material properties are E_b=4865N/mm^2, n_b=0.09 for the brick and E_m=1180N/mm^2, n_m=0.06 for the mortar joints.

A perfect plasticity assumption has been made for the mortar, with a tensile strength of 0.9N/mm^2. The brick is considered linear.

Figure 4. Mesh of the masonry RVE in COMSOL

4. The overall multi-scale computational homogenization scheme

A multi-scale computational homogenization model has been created with MATLAB, for the simulation of some masonry macroscopic structures.

The main idea of the present work, is to replace the simulation of an RVE in each Gauss point and each time step of the macro model, with the usage of the strain-stress and strain-stiffness database, which were created in the previous steps. By adopting this procedure, the method should become faster, as instead of solving a FEM microscopic problem in each Gauss point and time step, the databases and some interpolation method are used in order to obtain the macro stress and the consistent stiffness of the Newton-Raphson method.

For any current value of the macroscopic strain, a stress and a stiffness should be found from the databases previously created. Thus, an interpolation method must be used, to obtain these quantities from the databases. In this work the MATLAB function "TriScatteredInterp" is used, however other possible solutions for the creation of the metamodel (interpolation) can be used, for instance by using Neural Networks.

Concerning stresses interpolation, each strain vector (3x1) corresponds to one average stress value. For the consistent stiffness (3x3), each strain vector corresponds to one consistent stiffness value.

5. Results and discussion

5.1 COMSOL RVE analysis

In this section some results concerning the average stress - average strain relation and the failure of the RVE will be presented.

In particular, COMSOL parametric analysis results in the development of non-linear stress-strain laws, as it is depicted in Figure 5.

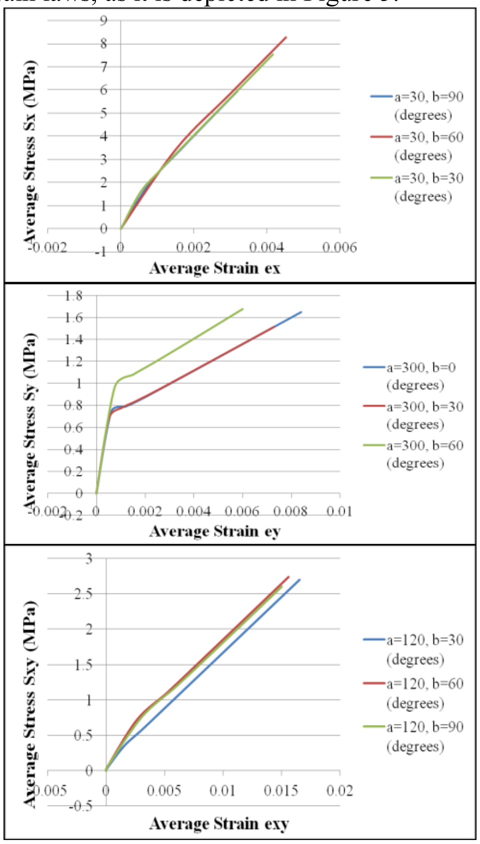
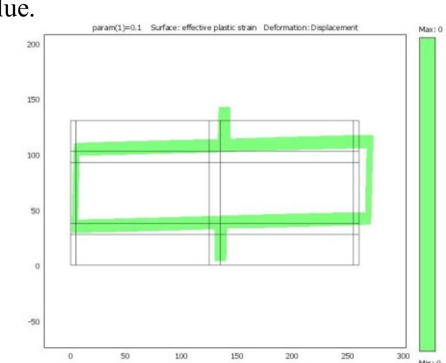


Figure 5. Average stress-average strain diagrams obtained from parametric COMSOL analysis

The failure mode of some RVEs is shown in Figure 6. According to these figures, plastic strains are developed only in the mortar joints. Moreover, as the parameter value is increased, the effective plastic strains given by COMSOL are also increased, from zero to a maximum value.



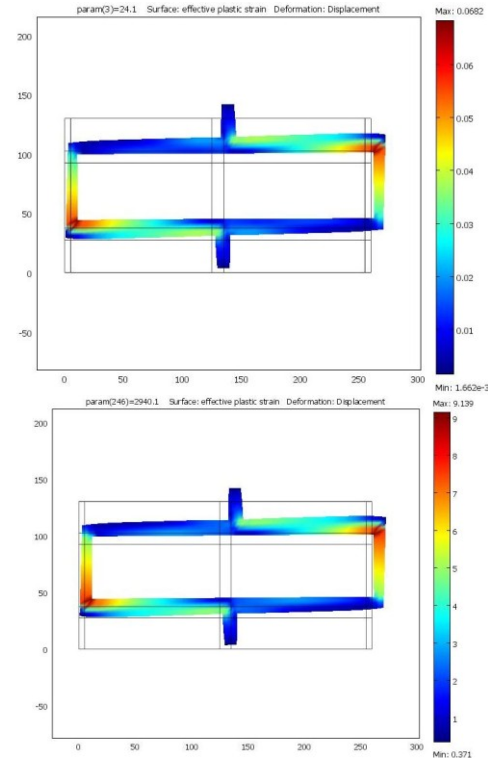


Figure 6. Effective plastic strain of the RVE, as the parameter of COMSOL analysis is increased

5.2 Multi-scale concurrent analysis results

The last step of the approach proposed in this article is related with the development of an overall FEM^2 numerical scheme for the study of macroscopic masonry structures. The results obtained from this approach are compared with the output received from commercial packages. In particular, ABAQUS and MARC have been used for the simulation of heterogeneous masonry structures, directly at the macroscopic scale (Direct Numerical Simulation, DNS models).

The first model which is presented here is a small rectangular masonry wall, with dimensions equal to 0.52x0.26m. Loading of this wall is a concentrated vertical load on the top-right corner of the model, while fixed boundary conditions are applied to the left vertical edge of it.

The force-displacement diagrams received from the two methods are shown in Figure 7.

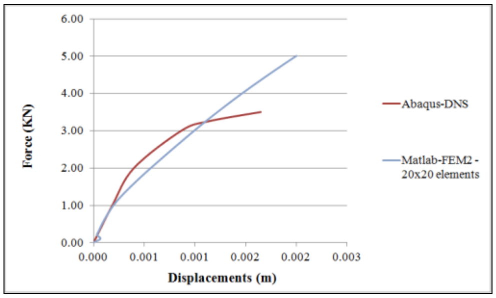
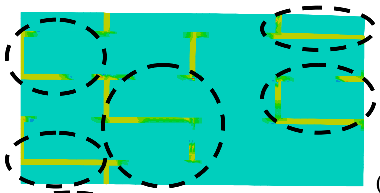


Figure 7. Force-displacement diagrams obtained from the proposed method and from a direct numerical macroscopic simulation

In Figure 8 a comparison of the failure modes obtained from the two approaches, is given. For the proposed FEM^2 approach the trace of the elasticity tensor has been calculated, as a qualitative measurement of the degradation of strength.


(a)

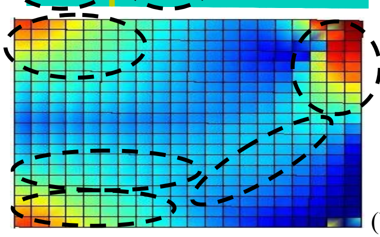
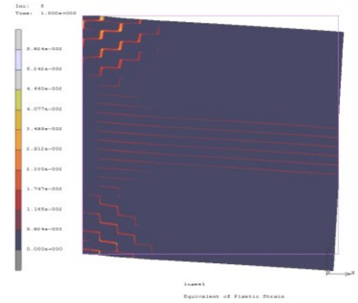
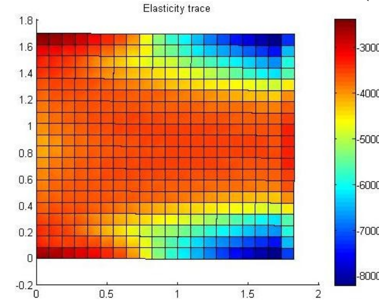

(b)

Figure 8. Degradation of the strength of a macroscopic masonry wall (a) ABAQUS direct macroscopic simulation (b) proposed FEM^2 approach

The dark blue color shows bigger values of trace, while the light blue which gradually becomes red, smaller values, respectively. The model received from ABAQUS uses the plastic strain distribution. With black circles some areas where failure is bigger, are located in the two domains.

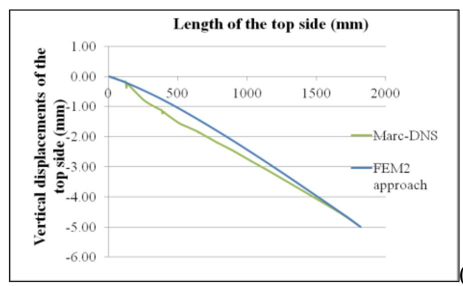
In Figure 9, a similar output is presented, for a bigger masonry wall, with dimensions 1.82x1.69m, fixed vertical left boundary and distributed displacements of 5mm at the right vertical edge, as loading. For the direct macroscopic simulation, MARC software has been used. According to this Figure, the degradation of the strength obtained from the two models, has the same distribution in the domain.


(a)

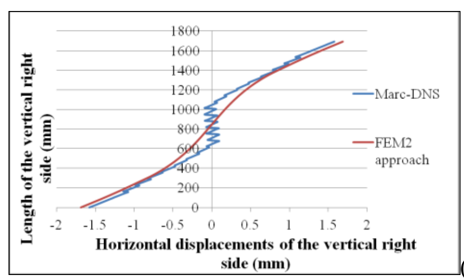


(b)

Figure 9. Degradation of the strength of a bigger macroscopic masonry wall (a) Marc direct macroscopic simulation (b) proposed FEM^2 approach



(a)



(b)

Figure 10. Distribution of (a) vertical displacements along the top side (b) horizontal displacements along the vertical right side, in the final time step

Finally, diagrams of Figure 10 indicate the distribution of the displacements in the top side and in the vertical right side of the structure, respectively. According to these diagrams, comparison between the two models leads to satisfactory results, indicating that the proposed approach can be used for the simulation of non-linear, heterogeneous structures.

6. Conclusions

A method for studying heterogeneous structures by taking into account the non-linear behaviour of them was proposed in this article. COMSOL Multiphysics was used to simulate with parametric analysis the non-linear RVE of a masonry structure. Then, the average strain, stress and stiffness were gathered and used in a FEM^2 approach, for the simulation of bigger masonry walls.

Results showed a good convergence with direct heterogeneous macroscopic models created with commercial FEM packages, indicating that the proposed method can be used for the investigation of heterogenous, non-linear materials. Among others, the force-displacement behaviour and the degradation of the strength were compared.

Finally, the method can be used with more accurate non-linear constitutive laws in the RVE and applied in more complex masonry structures, probably in three dimensions.

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