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NEW WAYS IN CONSTRUCTION MATERIALS MODELLING USING COMPUTER-AIDED ANALYSIS

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Abstract: *There has been a distinguished interest in understanding and simulating the behaviour of inhomogeneous materials (or composite materials in particular) for a significant amount of time. The fast development of computing technologies and the necessity of the development of unconventional and durable materials, the increased production and the crisis of the raw materials sources all call for new ways and possibilities for analysing and developing materials. This research aims to study the application of analytical and numerical methods through the newest computer software and discusses several modelling techniques to improve efficiency in computing the properties of inhomogeneous materials.*

Key words: *inhomogeneous materials, semi-analytical homogenization method, finite element method, Mori-Tanaka.*

1. Introduction

Theories on predicting and understanding the behaviour of different kinds of engineering and inhomogeneous materials were developed and improved over the time, starting with the numerical methods such as the Finite Element Method (FEM) as well the various homogenization methods.

Any homogeneous material can be considered an inhomogeneous one at a certain scale or a composite made up of a matrix with inclusions embedded in it, whether they are voids, particles, fibres or other constituents. [6]

Some techniques that allow for quick and cost-efficient analysis play an important role in material simulation and computational modelling. Of course, any simulation and modelling, whether numerical or analytical analysis, computer-aided or not, is based on tests and practical investigations and does not replace traditional tests. Their purpose and role in engineering is to facilitate the understanding of the behaviour of the analysed system, as well as optimization and cost reduction. Generally, in the field of material engineering, concept modelling involves multiscale analysis which occurs on at least two levels, from meso-, micro- or even nano-scale to macro level (full system), as shown in the figure below (Figure 1). [1]

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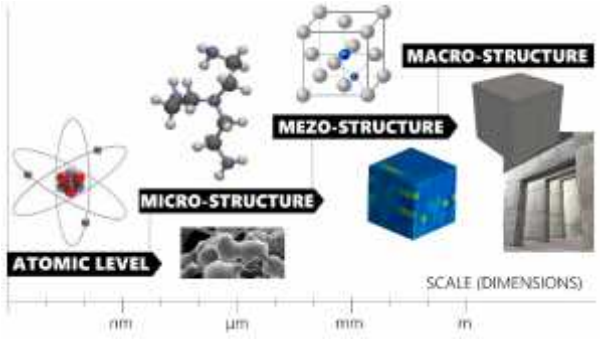


Fig. 1. *Multi-scale analyses in material engineering*

In the field of computer-aided engineering and materials technology, the latest trend is combining micromechanical theory with numerical methods. This kind of approach helps engineers study the behaviour of various materials with different kinds of constituents which help reduce development costs and time, resulting in innovative and high-quality materials. [1][3]

In this regard, the Digimat 2016 software, developed by e-Xstream Engineering (MSC Company), was studied and used. This research presents and examines the two different prediction approaches available for analysing inhomogeneous materials in this software. One such method is computer homogenization, based on nonlinear semi-analytical homogenization theory and the finite element method, which has been in use since the 1970s in several engineering applications. Thus, the software is divided into two different tools: Digimat-MF, based on homogenization methods, and Digimat-FE using FEM for analysis. Both of them are aimed at predicting the nonlinear thermomechanical behaviour of the heterogeneous materials. The main differences and the tools workflow presented in [3] are shown in Figure 2.

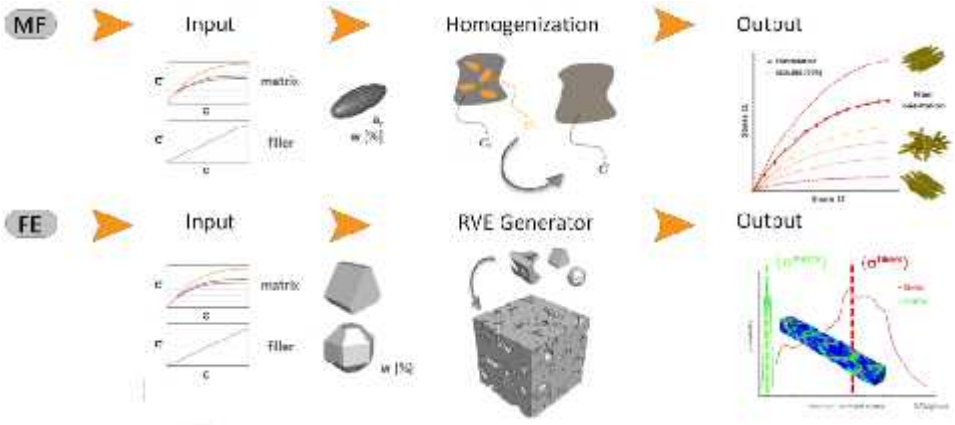


Fig. 2. *Digimat-MF vs. Digimat-FE workflow overview*

While Digimat-FE investigates the composites in-depth with 3D RVE, Digimat-MF represents a property screening approach, according to [3].

This paper also highlights the theoretical background of multi-scale material modelling, with particular emphasis on the most efficient homogenization methods.

2. Theoretical Background

In the case of virtual testing and development of materials using computational approaches, a representative volume element (RVE) is built, reproducing the appropriate material models assigned to each phase. This element can be viewed as a small sample cut from the material. It is typically used in micromechanics, for modelling inhomogeneous materials with a volume size large enough to include all heterogeneities in order to obtain a homogenized response of the material. [8][2]

One of the most commonly used approach in the field of material engineering and structural analysis in civil engineering is based on FEM.

Taking into account the advantages offered by the computing technologies and their fast development, this method allows us to simulate material microstructures with complex morphologies and non-linear behaviour. This method can highlight localized deformations through the concept of the RVE. There are many ways to simulate a realistic and complex geometry, depending on the software and the computer capacities used.

The essence of FEM computational modelling is a procedure called meshing, which consists of the continuous domain discretization of the RVE into discrete sub-domains and the solving the problem at hand with a set of partial differential equations. The first step is material geometry modelling, then specifying the properties of the material, as well as the boundary and loading conditions. The latter play a decisive role in solving the simulation. Inputting these conditions can easily be done using commercial pre-processors, and is facilitated by graphical user interfaces. [4]

A more efficient way from a computational point of view in order to analyse heterogeneous or composite materials is using homogenization methods. This approach also takes into account the interaction of the constituent phases and their individual properties and helps predicting the stress-strain behaviour and calculation of engineering properties, such as Young's Modulus and Poisson's ratio.

Generally, based on the Mean Field Theory, homogenization represents the determination of macroscopic or effective properties of the heterogeneous materials, based on the analysis of RVE, and is calculated as the averages of the corresponding micro fields. In consequence, the purpose of this approach is to predict the interaction between the macroscopic (effective) properties and the scale below it (meso- or in some cases microscopic properties). [8][7][5]

The different levels (e.g. macro, micro or meso level) can be linked by averaging methods, i.e. using homogenization techniques through the RVE (Figure 3).

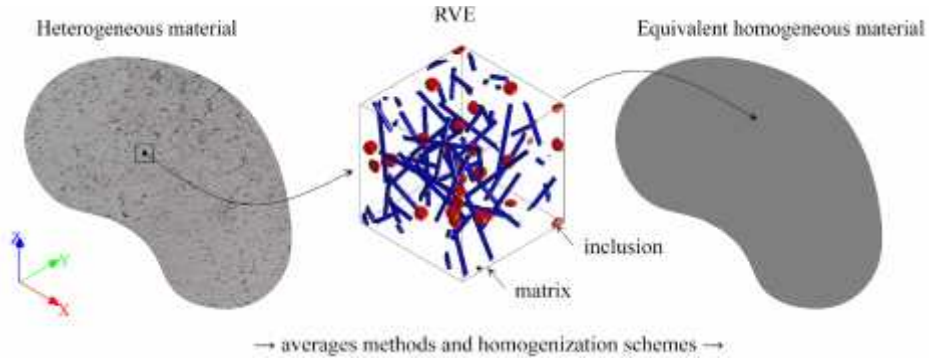


Fig. 3. *Representation of the micro (meso) – macro transition through the RVE concept*

It is assumed that the macroscopic properties of the analysed material are equal to the average mechanical properties of the established RVE, based on the material morphology, physical parameters and individual material engineering constants. In terms of stresses and strains, the concept can be formulated as follows:

$$\bar{\sigma} = \langle \sigma \rangle_{\mu} = \frac{1}{V}\int_{\mu} \sigma dV; \qquad \bar{\varepsilon} = \langle \varepsilon \rangle_{\mu} = \frac{1}{V}\int_{\mu} \varepsilon dV \tag{1}$$

where $\langle\ \rangle$ denote the average of the stress and the strain field over the RVE (domain and μ volume V), respectively. [1][3]

These equations do not solve the problem of homogenization, namely the equivalence of the inhomogeneous volume with a homogeneous one. In order to connect the average of stress/strain fields of the constituent phases, fourth-order concentration tensors were established and introduced. The homogenization models and schemes, such as Eshelby's solution, Mori-Tanaka or Double-Inclusion, differ from each other in establishing and determination of these tensors. In mathematical terms this can be formulated as:

$$\langle \sigma \rangle_{\mu_k} = \mathrm{A}_k \langle \sigma \rangle_{\mu}; \qquad \langle \varepsilon \rangle_{\mu_k} = \mathrm{B}_k \langle \varepsilon \rangle_{\mu} \tag{2}$$

where A and B are the fourth-order concentration tensors.

In the used software, two homogenization schemes are avaible: Mori-Tanaka (M-T) and Interpolative Double Inclusion (D-I). According to [1] the M-T model is very successful in predicting the effective properties of two-phase composites, with a restricted volume fraction of inclusions (less than 25%) while the D-I model usually gives excellent predictions of effective properties over all ranges of inclusions volume fractions, aspect ratios and stiffness contrasts (ratio of inclusions to matrix stiffness). This assumption was tested and the results were compared by the authors using Digimat-MF, presented in the next chapter.

3. Application of the Methodology

3.1. Material Modelling

This chapter focuses on analysing several material models using the methods presented in the previous section, through the Digimat Software Tools. A fictitious material with randomly oriented and distributed particles with high contrast in properties was chosen in order to highlight the differences and the efficiency of these methods.

Using the Digimat software, forces can be static and/or dynamic. In this study, mechanical uniaxial loads were applied in order to determine the primary elastic properties of the fictitious material.

Also, two shape types for inclusions were used to demonstrate the deficiency of homogenization-based methods and show a major difference compared to FEA. While an FE model allows the use of almost any shape in order to model the inclusions, MF approximates the inclusions with spherical shapes. This test highlights the influence of the inclusions shape as well. Depending on the property of the material, the constitutive law

model can be elastic, meaning that the deformation in the material disappears fully if it is unloaded, elastoplastic with or without damage, hyperplastic (in case of rubbers) etc.

Boundary conditions or the interface are another important consideration in materials modelling. As for the boundary condition, according to [3], periodic boundary conditions usually lead to the best predictions when compared to the Dirichlet and Mixed boundary condition type in Digimat. It also shows a faster convergence rate as the size of the volume element increases.

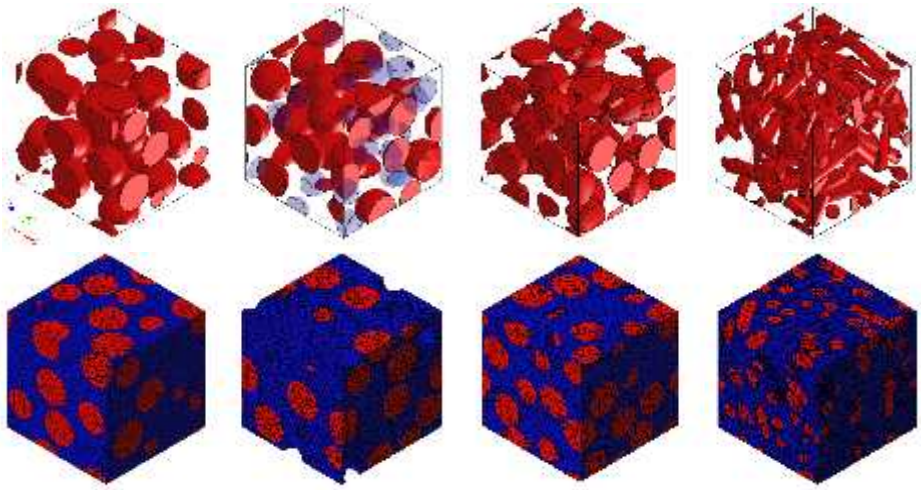
In the case of the homogenization method, the interfaces between components can only be perfectly bonded, although in reality this is not the case. However, it is possible to introduce an interfacial zone between the inclusions and the matrix with weaker properties, a phenomenon that occurs in the case of composite materials. Using the FE module or the FEM in general, different solutions exist in order to simulate the bounding between the phases.

This is not the single disadvantage of the MF module. While the FE module gives the Young's modulus value depending on the direction, the MF gives just a single, global value. Of course this is valid only in the case of isotropic materials.

Another very important feature of the Digimat software tools is the possibility of introducing voids in the material structures (Figure 4). It is a phase without stiffness or mechanical strength or properties. This way it is possible to simulate the influence of the material (matrix) porosity. Table 1 provides the input data for the software and shows the properties of the model created.

Material modelling – input data Table 1

Materials	**Volume fraction**	**Aspect ratio** [-]	**Elastic modulus** [MPa]	**Poisson's ratio** [-]	**Yield strength** [MPa]
Phase 1 (matrix)	60 %	-	20 000	0.2	11
Phase 2 (inclusion)	40 %	1	50 000	0.3	-



(a) 41558 elements; (b) 146502 elements; (c) 47344 elements; (d) 366207 elements.

Fig. 4. *Digimat-FE model: 3D RVE geometry and tetra type mesh (a) M1 – Two phase composite; (b) M2 – Three phase composite: considering 5% porosity; (c) M3 – Icosahedron shape; (d) M4 – Cylindrical shape.*

The first model (M1) was built by considering just the two phases: a matrix with elastoplastic constitutive law model and inclusions with spherical shape and elastic behaviour (properties presented in Table 1). Another three models were built: M2 – considering a matrix of 5% porosity, M3 – choosing an icosahedron (20-face polyhedron) and M4 – cylinder shape for the inclusions in the FE model to show the influence of the edges/shape on the composite properties.

The mesh type in the case of the FE model was automatic, considering that a complex model with different curve-shaped inclusions (e.g. spherical shape) cannot be meshed using voxel (brick) meshing (valid for the studied software). The RVE models generated in the FE model and meshes are shown in Figure 4.

3.2. Results and Discussions

The computer simulation results are shown in Table 2, Table 3 and Figures 5-8.

In the case of Digimat-MF, considering the three phase composite (M2): matrix, inclusion and voids, the software does not give directly the elastic properties of the material. This values, presented in Table 2 were calculated manually from the compliance matrix.

Material modelling – The elastic modulus of composites [MPa] Table 2.

Model	**Mori-Tanaka**	**Double-Inclusion**	**FEM** E1	**FEM** E2	**FEM** E3
M1	28316.0	28741.0	26191.8	26280.8	26307.9
M2	26095.3	*	24910.0	24802.5	24951.2
M3	**	**	25991.8	25928.4	26016.0
M4	28483	28854	23775.7	23794.7	23955.3

** Double Inclusion homogenization scheme cannot be used with void inclusions.*

*** Only spherical shape can be used for inclusions modelling.*

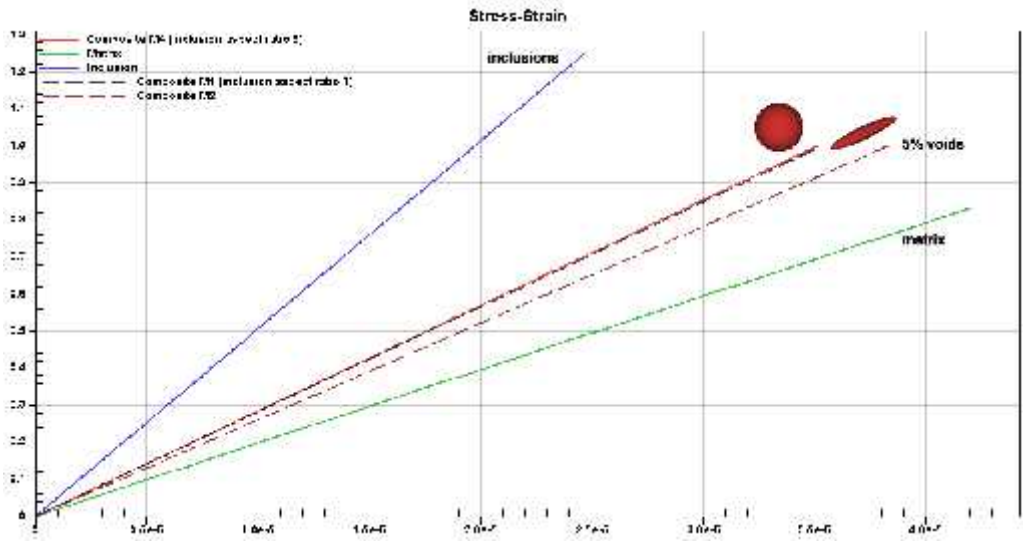


Fig. 5. *Digimat-MF results: Stress-Strain diagram. M1, M2 and M4 (Mori-Tanaka)*

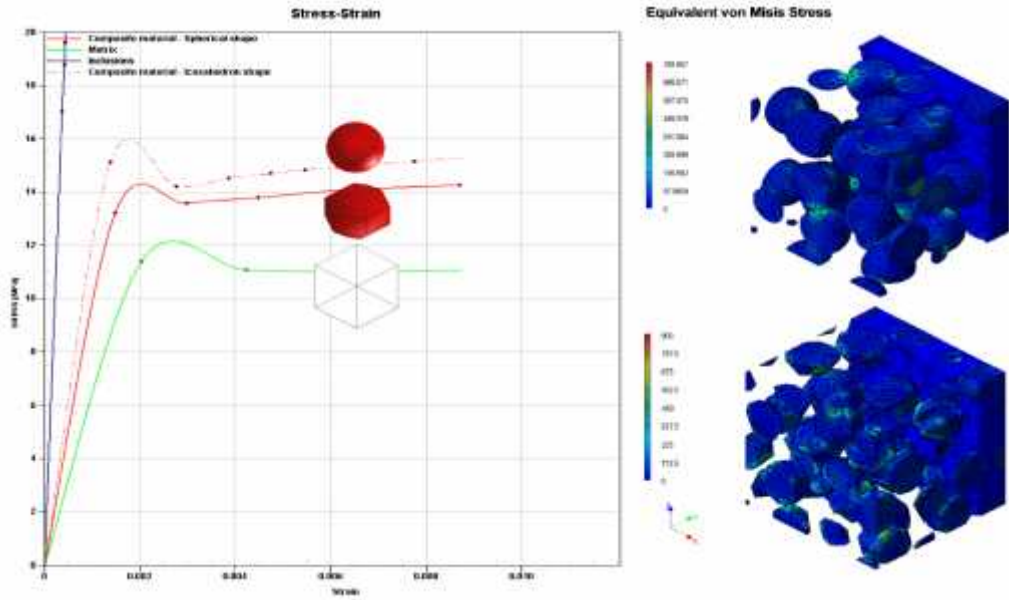


Fig. 6. *Digimat-FE results: the influence of the edges/shape on the composite properties. M1 and M3 models. The RVE's Stress-Strain diagram and Equivalent von Misis Stress*

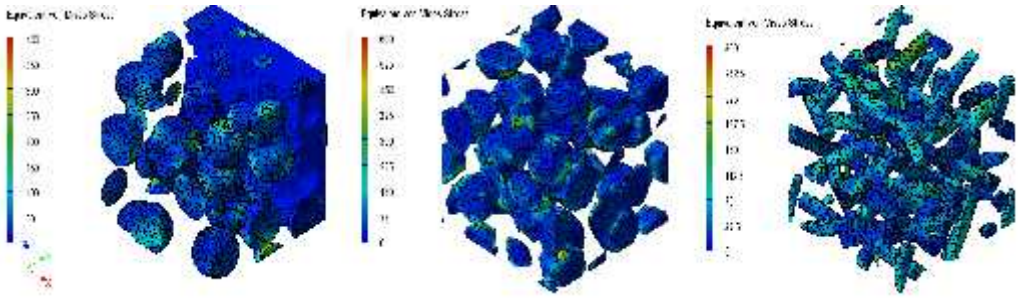


Fig. 7. *The three type of inclusions' shape under uniaxial loads. Equivalent von Mises stresses*

While in the case of MF the shape (aspect ratio) of the inclusions does not produce a major difference in strength or elastic properties (M1 and M4), in the case of FE a significant difference can be observed, according to Table 2 and Figures 5-6. The lowest increase of the yield strength (17.52%) has been achieved in the case of cylindrical shape (M4) compared to spherical (37.46%) or icosahedron (21.81), using FE.

Also to be mentioned that a 5% of porosity (M3) reduced the yield tensile strength by 8.7% compared to M1.

4. Conclusions

A benefit of computational approaches and modelling, and that of FEM in particular, is the load transfer simulation and highlighting between the constituent phases, the inclusion effect (distribution, orientation, size, shape etc.) on the matrix properties without costly

experiments. Naturally, this does not replace the laboratory investigations, but it is a good benchmark and can be used additionally for reducing the number of the specimens or as a preliminary test in choosing the composite's constituent materials.

In FE we have full control over the RVE (microstructure): size (distribution), shape, position, clustering, orientation, interpenetration etc., and generate a realistic 3D RVE. Using the homogenization method, the shape of inclusions can be approximated by the spherical shape aspect ratio.

As mentioned, the computational FE method gives detailed analysis of the material, while the MF gives less information about the material. With FEA we can analyse the local behaviour and local stresses of the RVE created, while by choosing MF we can approximate the increase of the material strength and the engineering constants. The global stiffness in this case does not depend on the applied load, but the MF is less time- and CPU-intensive. It takes only a few seconds compared to FEA, which takes from a few hours even up to days, depending on the complexity and size of the RVE, the type and the size of the mesh etc. It should be mentioned that the construction of the model and the RVE can be very difficult, but the software used in this study, the FE tool in particular, can simplify and reduce the duration of this task.

The studied software and approaches can be a significant advantage in the testing and modelling of construction materials. They allow for the optimization of mixtures and the preliminary components choice (before laboratory testing) by modelling different composites.

Also to be mentioned that the accuracy of the predictions cannot be studied using fictitious materials, but the findings of this research can be the basis of a future study which aims to investigate the accuracy of computer simulations as compared to laboratory test results.

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