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Response Surfaces in the Numerical Homogenization of Non-Linear Porous Materials

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The paper deals with the numerical homogenization of structures made of non-linear porous material. The material non-linearity causes a significant increase in computational costs for numerical homogenization procedure. The application of the response surface methodology allows for a significant reduction of the computational effort providing good approximation precision. Finite element method commercial software is employed to solve a boundary-value problem in both scales. Due to the significant reduction in computing time, the proposed approach may be applied for different optimization and identification tasks for inhomogeneous, non-linear media, especially with the use of global optimization methods.

Key words: numerical homogenization; response surface; porous material; non-linear material.

1. Formulation of the problem

Porous materials are an important group of inhomogeneous structural materials. Their macro properties depend on such microscale parameters as the porosity and shape and the location of voids at micro scale [1]. A large popular group of porous media are porous metallic materials, like porous Al, Ti, Mg and others. They are characterized by outstanding mechanical, electrical, thermal and acoustic properties while maintaining a low density [2]. Porous materials are applied as structural elements, e.g. in grinding wheels, metal self-lubricating bearings, gas-permeable moulds, surgical implants and impact energy absorbers [3].

The behaviour of inhomogeneous material can be described by differential equations with discontinuous coefficients, like elastic constants for linear-elastic materials. To obtain the macroscopically homogenous, equivalent effective continuous coefficients of differential equations, numerical homogenization is performed [4].

Many inhomogeneous materials, like composites or porous materials, exhibit physically non-lineal behaviour. The aim of the paper is to develop an efficient approximate numerical homogenization procedure for inhomogeneous structures. As it is assumed that the material is non-linear, the incremental procedure is involved, which dramatically increases the computational effort. The main idea is to replace the full non-linear homogenization procedure for isotropic materials by initial analyses of the representative volume elements and to determine the relationship between stresses and strains in the form of a response surface. The proposed approach significantly reduces the computational cost of the homogenization procedure with an acceptable decrease in its accuracy.

Presented methodology may be especially useful in different multi-scale optimization and identification problems for non-linear materials. As such problems are often multimodal, global optimization algorithms should be applied. Global and usually populational optimization methods, process a set of potential solutions in one iteration and they are time and memory demanding (comparing, e.g. with gradient-based optimization methods) [5]. Authors' applications of bio-inspired global optimization methods for multiscale optimization and the identification of structures made of linear materials are presented, e.g. in [6, 7] and [8].

ANSYS DesignXplorer software is employed to construct and verify response surfaces [9]. Finite element method software is applied to solve the boundary-value problem in both considered scales [10].

2. Numerical homogenization

Different inhomogeneous materials in form of composites and porous materials are widely applied in modern industry. To predict the behaviour of such materials considering more than one scale it is necessary to create a proper model. Direct multiscale modelling of the whole inhomogeneous structures leads to an enormous number of equations to solve. Homogenization methods make it possible to obtain a medium macroscopically equivalent to an inhomogeneous medium in a micro scale [11]. The effective properties od homogenized material may be obtained using analytical, empirical or computational methods. Diverse procedures applied for the homogenization of porous linear and non-linear media are described, e.g. in [12] and [13].

A typical approach to different homogenization methods relies on the idealisation of microstructural heterogeneities and the simplification of the spatial distribution of inclusions. The problem consists in the determination of a representative volume element (RVE) on which averaging is performed, on the selection of boundary conditions and on the construction of numerical models of its heterogeneity, assuming local periodicity [14].

Numerical homogenization methods, also known as local-global analysis, allow for the determination of the stress-strain relation at any point of the structure through precise modelling of microstructure at this point. Numerical (computational) homogenization methods involve the examination of finite-sized volume elements containing a detailed distribution of material inhomogeneities.

The most common approach to the numerical homogenization is the determination of a constitutive relation between averaged field variables, like stresses or strains [15]. Different numerical methods may be used to perform the numerical homogenization, e.g. the finite element method (FEM) [16] or the boundary element method (BEM) [17]. In the present paper, FEM software is employed to perform numerical homogenization.

2.1. Numerical homogenization of linear materials

It is assumed that the RVE fully represents the behaviour of the whole material or its part [18]. In this case the following conditions must be satisfied for RVE of the volume V:

a) the RVE characteristic dimension is relatively small comparing to the macroscale dimensions and relatively large comparing to the micro-scale dimensions (separation of scales),

b) the equality of the average energy density at a micro scale and the macroscopic energy density at the macrostructure point corresponding to the RVE (the Hill-Mandel condition):

$$\langle \sigma_{ij}\varepsilon_{ij}\rangle = \langle \sigma_{ij}\rangle \langle \varepsilon_{ij}\rangle , \tag{2.1}$$

where σ_{ij} – micro stress tensor, ε_{ij} – micro strain tensor, $\langle\cdot\rangle$ – the averaged value of the considered field:

$$\langle\cdot\rangle = \frac{1}{|V|}\int_V (\cdot)\,\mathrm{d}V, \tag{2.2}$$

c) boundary conditions satisfying Hill-Mandel condition, usually in one of the forms:

– uniform traction (the Reuss assumption):

$$t_j|_{\partial V} = \sigma_{ij}n_i \Rightarrow \langle \sigma_{ij}\rangle = \sigma_{ij}, \tag{2.3}$$

– uniform displacements:

$$u_j|_{\partial V} = \varepsilon_{ij}x_i \Rightarrow \langle \varepsilon_{ij}\rangle = \varepsilon_{ij}, \tag{2.4}$$

– periodic boundary conditions:

$$u_j^+ - u_j^- = \langle \varepsilon_{ij} \rangle \cdot \left(x_i^+ - x_i^- \right), \qquad t_i^+ = -t_i^-, \qquad \forall \mathbf{x} \in \partial V : n_i^+ = -n_i^-, \tag{2.5}$$

where u_j – displacements, t_i – tractions, x_i – coordinates of points on RVE boundary ∂V, n_i – components of the vector normal to the boundary ∂V.

If FEM is used to solve the boundary-value problem in both scales, RVEs are associated with each integration point on the macro scale. In addition to periodic boundary conditions, deformation boundary conditions from a higher scale (localization) are imposed on each RVE. As a result, average stresses (homogenization) are obtained for RVE, which are transferred to a higher scale and are used to determine homogenized values of material parameters on a macro scale.

Assuming the zero-displacement field within the pores, averaged strain and stress tensors for porous material may be calculated as [19]:

$$\langle \varepsilon_{ij} \rangle = \frac{1}{|V|} \int\limits_{V_m} (\varepsilon_{ij}) \, \mathrm{d}V + \left\langle \varepsilon_{ij}^c \right\rangle, \qquad \langle \sigma_{ij} \rangle = \frac{1}{|V|} \int\limits_{V_m} (\sigma_{ij}) \, \mathrm{d}V, \tag{2.6}$$

where ε_{ij}^c – the cavity strain due to the deformation of the boundary of the pores, V_m – the RVE matrix volume.

The constitutive equation for linear-elastic homogenized material can be expressed as:

$$\langle \sigma_{ij} \rangle = Q_{ijkl} \langle \varepsilon_{ij} \rangle, \tag{2.7}$$

where Q_{ijkl} – stiffness tensor, i, j, k, $l = 1, 2, 3$.

2.2. Numerical homogenization of non-linear materials

For linear analyses, the one-way information transfer (from micro to macro scale) of averaged field values is sufficient. Otherwise, a two-way information transfer is necessary. In contrast to linearly-elastic models, non-linear materials' homogenization tasks are much more time and memory requiring, due to the necessity of solving a large number of local models and keeping information of stress/strains distributions for all RVEs. Solution of non-linear problems is related to the iterative approach, like Newton-Raphson or arc-length methods [20].

During the task solving, the values of external loads and internal forces resulting from non-linear material behaviour are analysed until specific convergence conditions are obtained. Due to local changes in the material structure caused, for example, by plasticity, a local RVE is introduced for each material point (the integration point in the macroscopic model) [21, 22]. At each iteration of the macroscopic task, the values associated with the strain tensor are transferred to the local RVE and the non-linear simulation is performed to determine the state of stress. The task is considered solved when the convergence of forces is met for the macroscopic model and each local RVE model.

3. Response surfaces methodology

To reduce the computational cost, the response surfaces methodology (RSM) strategy is proposed. Response surfaces, also known as metamodels, surrogates, emulators or auxiliary models are simplified models of an actual models. They approximate the input-output function that is implied by the underlying simulation model [23]. RSM is a collection of mathematical and statistical techniques useful for problems in which a few independent input variables influence the response of interest (performance measure). Such techniques are helpful in developing, improving and optimizing processes [24].

As in the most RSM problems the real response function is not known, it is necessary to develop a proper approximation of the response function and control some parameters describing its quality [25].

The RSM is often applied to reduce the computational effort as it provides almost instantaneous output parameters by approximate evaluation. A high accuracy of the response function may be obtained for several design points only. To control the quality of the response surface, different metrices are introduced. In the typical approach, the calculation of the response function (functions) starts from a small number of points and the correctness of the obtained approximation is verified for selected verification points. If its quality is unsatisfactory, the refinement points are introduced to modify the response surface.

There are several approaches to create response surfaces, e.g. 1st and 2nd order polynomials, Kriging, non-parametric regression, genetic aggregation or artificial neural networks. In the present paper the non-parametric regression (NPR) is employed to create a response surface. Such method is especially convenient for nonlinear responses with noisy results [9]. In NPR method, the margin tolerance ε creates an envelope around the actual output surface and all (or most) of the sample points.

NPR belongs to a class of Support Vector Method (SVM) type techniques in which hyperplanes are used to separate data groups [26]. The response surface is approximated as:

$$f(\mathbf{X}) = \langle \mathbf{W}, X \rangle + b = \sum_{i=1}^{N} (A_i - A_i^*) \cdot K(\mathbf{X}_i, \mathbf{X}) + b, \tag{3.1}$$

where $\mathbf{W}$ – a weighting vector, $\mathbf{X}$ – an input sample, b – a bias, A – Lagrange multipliers, K – radial basis functions, N – the number of sample points.

The Lagrange multipliers are the unknown parameters and a pair A_i and A_i^* is defined by tolerance values ε^+ and ε^- respectively for each input variable. The Lagrange multipliers are calculated by minimization of the weight function.

4. Response surfaces in numerical homogenization of non-linear materials

In the proposed methodology, the response surfaces are generated on the basis of the selected input parameters for a relatively small number of training data.

At the beginning, the limits for the input parameters (such as porosity and stress tensor components' values) are set and the initial number of training data necessary to prepare the response surface is taken. For each training point, a proper RVE is created and appropriate boundary conditions are applied. In the first homogenization step, linear simulation is performed, and reaction forces values are calculated. On the basis of the reaction values, equivalent Young's modulus and Poisson's ratios are calculated.

In the second homogenization step, non-linear, incremental analysis is performed for given RVEs. The results in the form of tractions allow for the computation of average stress values as the function of input parameters. The response surface generated based on the obtained results describes the dependence of stresses on porosity and strain tensor values.

The quality of the response surface is controlled by means of 4 selected metrices: coefficients of determination (R^2 measure), adjusted coefficient of determination, maximum relative residual and root mean square error [13]. If the quality of the answer surface is not high enough, the number of training data increases and the whole procedure is repeated for additional training points.

As the values connected to stress distribution obtained for macroscopic model simulation are the averaged ones, additional steps are required to calculate the real values of stresses. To calculate the local stress distribution, it is necessary to perform the sub-model analysis for the RVE located in selected point(s).

The block diagram of the proposed methodology is presented in Fig. 1.

The received response surface can be used as a set of material input information for macroscopic simulation of heterogeneous materials, also considering the non-uniform distribution of microstructure parameters (e.g. gradient materials).

The simulation based on the response surface makes it possible to obtain displacement results and an approximate average stress state without performing local RVE analysis for each integration point of the structure. The proposed methodology also allows for fast and fairly accurate determination of critical places in the structure as well as a calculation of the permissible load.

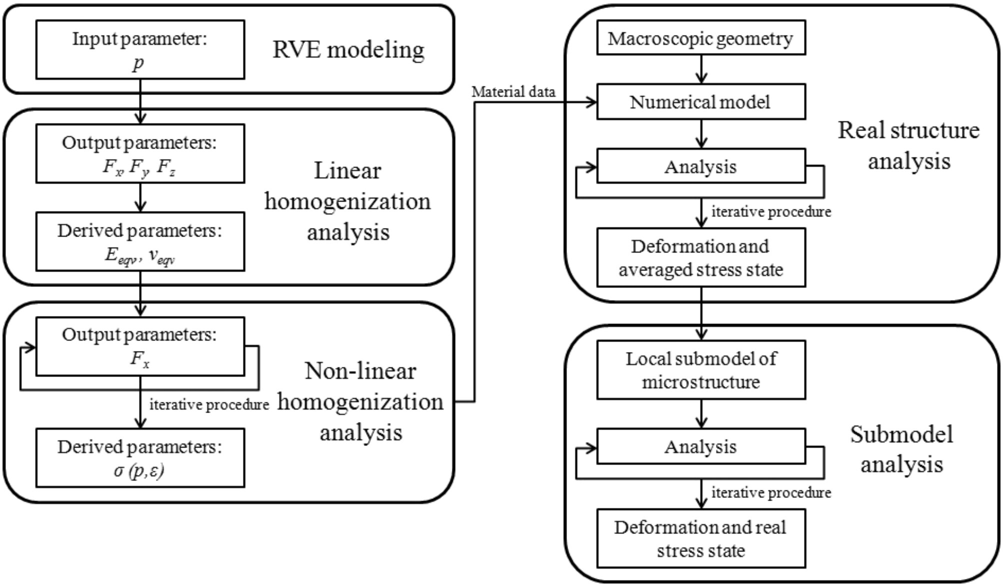

Fig. 1. Block diagram of numerical homogenization with the use of response surfaces.

5. Numerical example

A porous material in the form of Ti-6Al-4V alloy with the porosity in the range $p = 0.01$–0.8 is considered. It is assumed that the material is nonlinear, and it is defined as a bilinear elastoplastic one. The material parameters for non-porous Ti-6Al-4V alloy are: Young's modulus $E = 113.8$ GPa, Poisson's ratio $v = 0.3$, yield point $R_e = 1.09$ GPa, strain hardening modulus $E_T = 0.85$ GPa, density $\rho = 4430$ kg/m^3.

It is assumed that RVEs contain 64 uniformly distributed spherical voids of different diameters for each considered porosity level. Exemplary FEM meshes for limit porosity values are presented in Fig. 2.

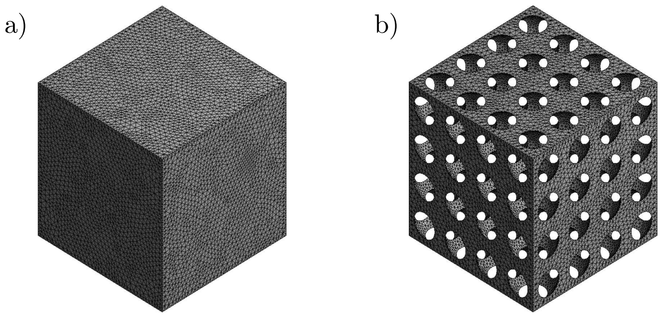

Fig. 2. RVE FEM mesh for porosity: a) $p = 0.01$ (96 170 Tet10 elements), b) $p = 0.8$ (158 847 Tet10 elements).

To obtain the response surface, linear and non-linear analyses are necessary. Two input parameters are introduced to the model: porosity p and the normal strain component ε. For each porosity level a linear simulation with displacement boundary conditions is performed – as a result, the reactions at the boundaries are calculated. In the next step, equivalent E and v values are calculated by means of the numerical homogenization procedure.

The non-linear tension is performed on the RVE which result in the averaged stress values for given p and ε. The procedure is repeated according to assumed experiment plan (here: 8 times). The obtained response surface is presented in Fig. 3.

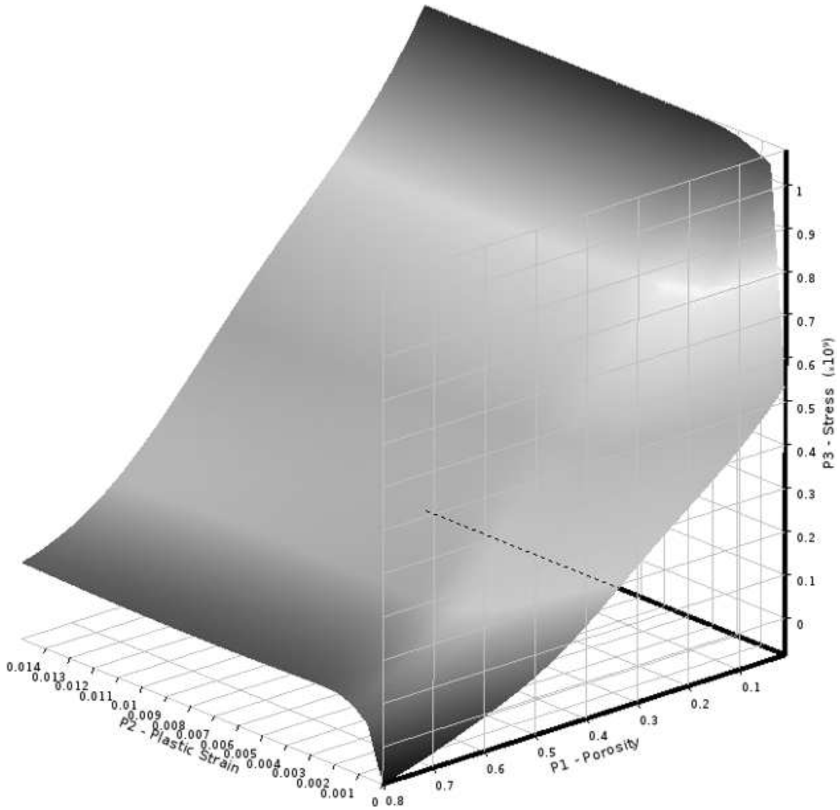

Fig. 3. Response surface for porous Ti-6Al-4V alloy.

The obtained response surface was used to perform the numerical homogenization of a real structure. A porous supported beam of dimensions $b \times h \times l = 20 \times 30 \times 100$ mm supported and loaded as presented in Fig. 4a is considered. It is assumed that the porosity $p = 0.2$. FEM mesh consists of 1250 20-node Hex20 hexahedral elements.

In the first step, the linear analysis was performed. As a result, the displacement values for the beam are calculated by means of the response surface strategy (Fig. 4b).

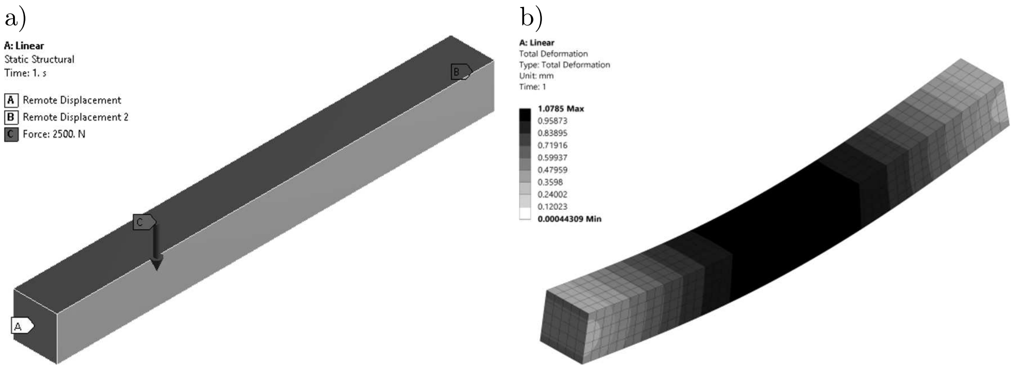

FIG. 4. a) The cantilever beam: loading and support and b) the FEM mesh and displacement map for linear material model.

An exemplary location of the RVE for the calculation of the local stress distribution is presented in Fig. 5. The displacement boundary conditions are transferred to microscopic model from the macroscopic one to perform the homogenization procedure.

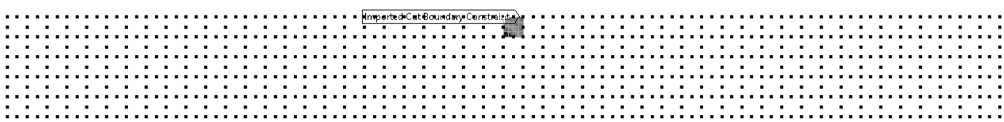

FIG. 5. The cantilever beam: an exemplary RVE location for local stress calculation.

The results in the form of the colour maps of total deformations and equivalent von Mises stresses are presented in Fig 6.

In the second step, the non-linear analysis of the beam was performed. The displacement of the whole structure and for the RVE located in the selected point are presented in Fig. 7.

The von Mises stress and plastic strain distributions for selected RVE are presented in Fig. 8.

To verify the procedure, the macroscopic model with 12 960 pores for non-linear analysis was considered. Three different discretization variants were considered.

A hardware configuration for homogenized, local RVE and global models are collected in Table 1.

It can be observed in Table 2 that the displacement value obtained for the homogenized model is similar to values obtained for non-homogenized macroscopic

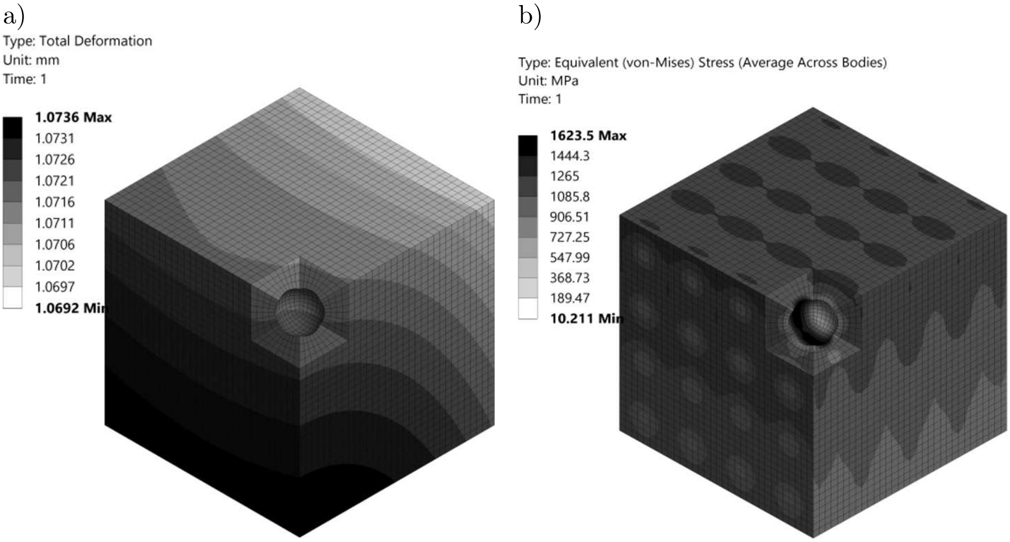

Fig. 6. RVE in selected location (linear material model):
a) total deformations, b) von Mises stresses.

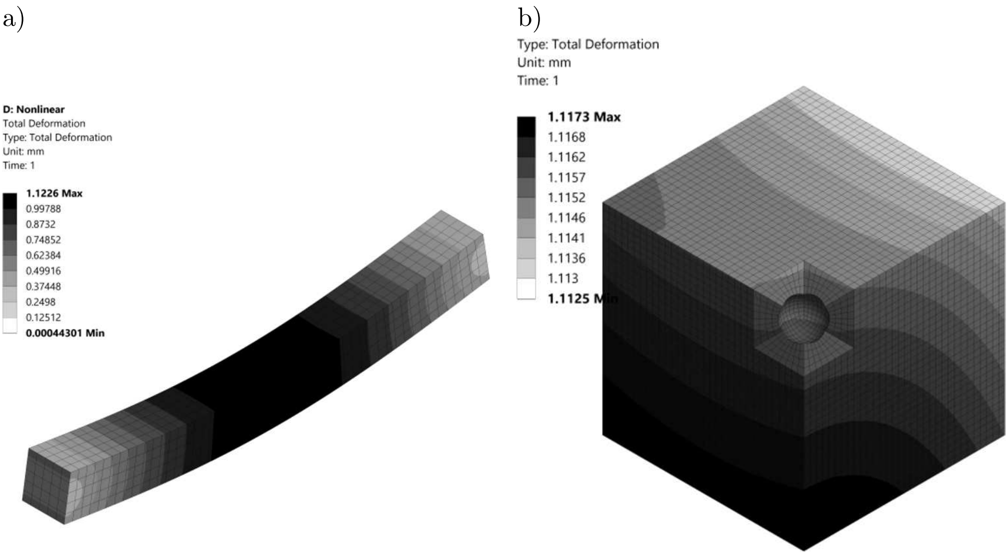

Fig. 7. Nonlinear material model – displacement maps for:
a) the whole beam, b) the RVE in selected location.

models. Moreover, if the discretization in the non-homogenized model is better (a higher number of elements or a better geometry approximation with hexahedral elements), the displacement values are getting closer to the homogenized model.

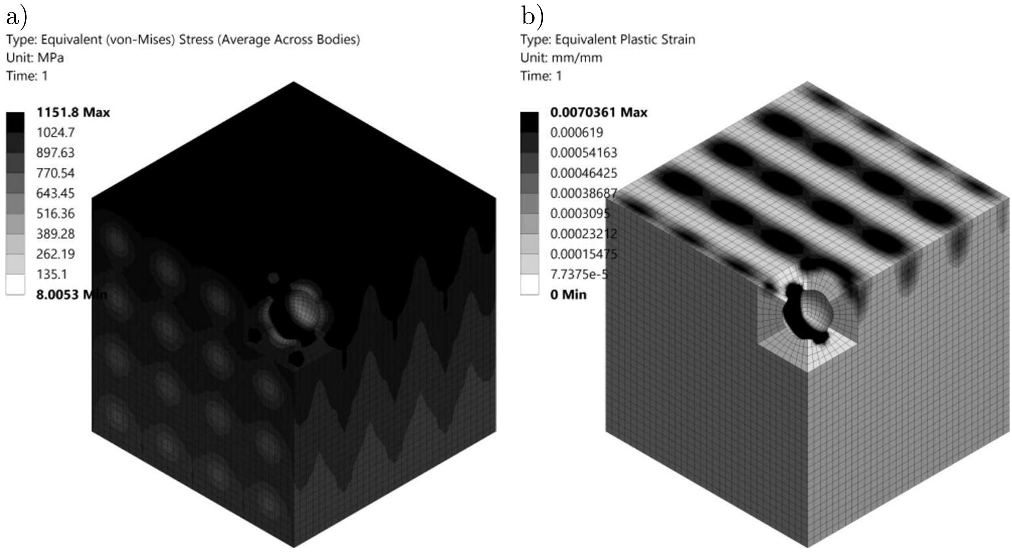

Fig. 8. Nonlinear material model, RVE results: a) von Mises stresses, b) plastic strains.

Table 1. Hardware configuration for different models.

Task	Homogenized and RVE models – desktop PC	Global models – HPC Workstation
No. of cores	4	8
Processor	Intel Core i7-4710MQ 2.5 GHz	Intel Xeon E5-2640 v3 2.6 GHz
RAM [GB]	16 GB	128 GB
Operating system	Windows 10	Windows 7

Table 2. Comparison of the computational effort for homogenized model, local RVE and global model.

	Surface resp. strategy	Local RVE	Global model 1	Global model 2	Global model 3
No. of nodes	6 696	437 505	5 729 086	14 320 207	21 804 020
No. of elements	1 250	98 304	3 889 568	9 901 175	4 860 000
Element type	Hex20	Hex20	Tet10	Tet10	Hex20
Max displacement [mm]	1.1226	1.1173	1.062	1.0792	1.09574
Max von Mises stress [MPa]	677.15 (averaged)	1151.8	1216	1226.4	1340.19
Max plastic strain [–]	6.19E-04 (averaged)	7.04E-03	4.60E-03	8.61E-03	1.46E-02
RAM usage [MB]	154	2 347	43 519	95 600	153 100
Analysis time [s]	7	127	1 888	9 409	25 428

The comparison of the results for nonlinear material model for: homogenized, local RVE and global models are collected in Table 2.

The maximum equivalent stress from RVE calculated by the homogenized model is smaller but the stress distribution is much more continuous than in non-homogenized ones, so the maximum values may be calculated incorrectly due to too coarse meshes. The application of fine mesh to such a model turned out to be too computationally expensive (RAM usage and acceptable analysis time).

The plastic strain values may be treated as calculated with the acceptable precision considering the overall time efficiency of the proposed approach.

6. Final conclusions

In the present paper an efficient way of the reduction of the computational effort in case of the numerical homogenization of the non-linear material has been proposed. Surface response methodology strategy allows for a significant reduction of computations necessary to obtain homogenized values of the state field in multiscale analysis of non-linear heterogeneous materials. The obtained results accuracy is satisfactory and analysis time has been considerably reduced. The type of the response surface has to be tailored to the problem. The quality of the response surface must be precisely controlled using suitable metrics to describe the mapped function properly. The presented numerical example shows the effectiveness of the proposed procedure.

Further research has to be performed to determine method effectiveness and accuracy for objects under multiaxial stress and non-linear strain state.

The presented methodology may be applied to multiscale problems for different inhomogeneous media with material nonlinearities, e.g. composites. Such approach is planned to be applied for different optimization and identification problems with non-linear and inhomogeneous materials.

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