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## ROBUST MULTISCALE MODELLING OF TWO-PHASE STEELS ON HETEROGENEOUS HARDWARE INFRASTRUCTURES BY USING STATISTICALLY SIMILAR REPRESENTATIVE VOLUME ELEMENT

### EFEKTYWNE MODELOWANIE WIELOSKALOWE STALI DWUFAZOWYCH NA HETEROGENICZNYCH ARCHITEKTURACH SPRZĘTOWYCH Z WYKORZYSTANIEM STATYSTYCZNIE PODOBNYCH REPREZENTATYWNYCH ELEMENTÓW OBJĘTOŚCIOWYCH

The coupled finite element multiscale simulations (FE<sup>2</sup>) require costly numerical procedures in both macro and micro scales. Attempts to improve numerical efficiency are focused mainly on two areas of development, i.e. parallelization/distribution of numerical procedures and simplification of virtual material representation. One of the representatives of both mentioned areas is the idea of Statistically Similar Representative Volume Element (SSRVE). It aims at the reduction of the number of finite elements in micro scale as well as at parallelization of the calculations in micro scale which can be performed without barriers. The simplification of computational domain is realized by transformation of sophisticated images of material microstructure into artificially created simple objects being characterized by similar features as their original equivalents. In existing solutions for two-phase steels SSRVE is created on the basis of the analysis of shape coefficients of hard phase in real microstructure and searching for a representative simple structure with similar shape coefficients. Optimization techniques were used to solve this task. In the present paper local strains and stresses are added to the cost function in optimization. Various forms of the objective function composed of different elements were investigated and used in the optimization procedure for the creation of the final SSRVE. The results are compared as far as the efficiency of the procedure and uniqueness of the solution are considered. The best objective function composed of shape coefficients, as well as of strains and stresses, was proposed. Examples of SSRVEs determined for the investigated two-phase steel using that objective function are demonstrated in the paper. Each step of SSRVE creation is investigated from computational efficiency point of view. The proposition of implementation of the whole computational procedure on modern High Performance Computing (HPC) infrastructures is described. It includes software architecture of the solution as well as presentation of the middleware applied for data farming purposes.

*Keywords:* multiscale modelling, high performance computing, AHSS.

Symulacje wieloskalowe z wykorzystaniem sprzężonej metody elementów skończonych wymagają kosztownych numerycznych procedur zarówno w skali makro jak i mikro. Próby poprawy efektywności numerycznej skupione są przede wszystkim na dwóch obszarach rozwoju tj. zrównoleglenie/rozproszenie procedur numerycznych oraz uproszczenie wirtualnej reprezentacji materiału. Jedną z metod reprezentującą obydwa obszary jest podejście Statystycznie Podobnego Reprezentatywnego Elementu Objętościowego. Głównym celem tej metody jest redukcja ilości elementów dyskretyzujących przestrzeń obliczeniową, ale również możliwość zrównoleglenia obliczeń w skali mikro, które mogą być realizowane niezależnie od siebie. Uproszczenie domeny obliczeniowej poprzez tworzenie elementu SSRVE realizowane jest za pomocą metod optymalizacji umożliwiających tworzenie elementu najbardziej podobnego do rzeczywistego materiału na podstawie wybranych cech charakterystycznych. W rozwiązaniu dla stali dwufazowych cechy opisujące podobieństwo są tworzone na podstawie analizy współczynników kształtu ziaren martenzytu na zdjęciu rzeczywistej mikrostruktury. Natomiast podejście przedstawione w niniejszym artykule zostało rozbudowane dodatkowo o lokalne wartości naprężeń i odkształceń tak, aby w pełni odzwierciedlić podobieństwo zarówno wizualne jak i behawioralne. Różne formy funkcji celu zostały poddane analizie w procesie optymalizacji, a uzyskane wyniki zostały porównane pod względem jakości, a także efektywności i unikalności rozwiązania. Ostatecznie zaproponowana została najlepsza funkcja celu obejmująca współczynniki kształtu oraz wartości naprężeń i odkształceń. Przykłady SSRVE wyznaczone dla analizowanych stali dwufazowych zostały przedstawione w artykule. Natomiast każdy krok procedury tworzenia elementu SSRVE został poddany analizie wydajności obliczeniowej, na podstawie której zaproponowane zostało podejście wykorzystujące nowoczesne architektury sprzętowe wysokiej wydajności. Opis podejścia zawiera zarówno architekturę rozwiązania jak i prezentację oprogramowania warstwy pośredniczącej.

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## 1. Introduction

There is a general need for an increase of a strength-to-density ratio of materials, in particular in the automotive and aeroplane industries. The former still uses steels for car body parts and intensive research is carried out on improvement of strength of steels. Maintaining good ductility while increasing the strength is an additional necessary condition. This research led to development of Advanced High Strength Steels (AHSS), in which multi-phase microstructure allows to improve both strength and plastic properties, see for example [1]. The strength/ductility balance was noticeably further improved with a new group of steels: high manganese steels with induced plasticity (X-IP, often called 2nd generation AHSS) [2]. Strain-induced twinning here leads to very strong work hardening. High level of alloying elements increases manufacturing costs of these steels and is not likely to be accepted by car industries, which manufacture millions of cars every year. This inspired scientists to search for methods of improvement of properties by specific thermal cycles leading to special morphology and improvement of properties of multi-phase steels, without changing the chemistry. As a consequence, 3rd generation AHSS with allowing elements below 10% were proposed in 2010. Intensive research in this field is still carried out and the objective is to improve properties by control of volume fractions, morphologies and properties of individual phases.

Numerical modelling can support this research but multiscale modelling techniques [3,4] have to be applied to supply data concerning mentioned above features of the multi-phase microstructure. Among various multiscale techniques those based on upscaling and Representative Volume Element (RVE) are the most suitable for the design of AHSS microstructure. The coupled finite element multiscale simulations (FE<sup>2</sup>) require costly numerical calculations, therefore, researchers are searching for methods of improving of efficiency of calculations in both macro and micro scales [5]. The idea of the SSRVE presented in [6] and developed further in [7,8] is one of possible solutions. It aims at the reduction of the number of finite elements in micro scale by transformation of sophisticated images of material microstructure into artificially created simple objects being characterized by similar features as their original equivalents. In the paper [9] analysis of shape coefficients and possibilities of their application in the creation of SSRVE for two-phase steels was discussed. Optimization techniques with the similarity of the shape coefficients used as the objective function were applied. It was observed, however, that shape coefficients alone do not guarantee obtaining the unique solution as far as representation of fields of strain and stresses in the dual phase microstructure is considered. Therefore, the current work is dedicated to accounting for the strain and stress distributions in the objective function in the optimization. Additionally, the part of the paper is devoted to aspects of parallelization and distribution of computational procedures, which became very important issue in various applications of numerical modelling [10]. The strategy of usage of HPC infrastructure is proposed in the paper.

## 2. Statistical representation of the microstructure

### 2.1 Idea of the SSRVE

The idea of the SSRVE is well described in [6,7,8] and it is repeated only briefly here. The objective is to develop the simple SSRVE, which will allow to decrease the computing costs and will make micro-macro modelling approach more efficient. Considering micro-heterogeneous materials, the continuum mechanical properties at the macro scale are characterized by the morphology and by the properties of the particular constituents in the micro scale. In the present paper two-phase microstructures composed of soft ferrite and hard martensite are considered.

An usual RVE is determined by the smallest possible sub domain, which is still able to represent the macroscopic behaviour of the material. Although these RVEs are the smallest possible by a definition, they still can be too complex for the efficient calculations. Therefore, the construction of statistically similar RVEs, which are characterized by a lower complexity than the smallest possible substructure, was proposed in [6]. The basic idea is to replace a RVE with an arbitrary complex inclusion morphology by a periodic one composed of optimal unit cells, see figure 1. The description of the microstructure is based on statistical consideration [11]. This idea is applied in the present work to the analysis of the two-phase steel microstructures. Strains and stresses are added as measures characterising the microstructure.

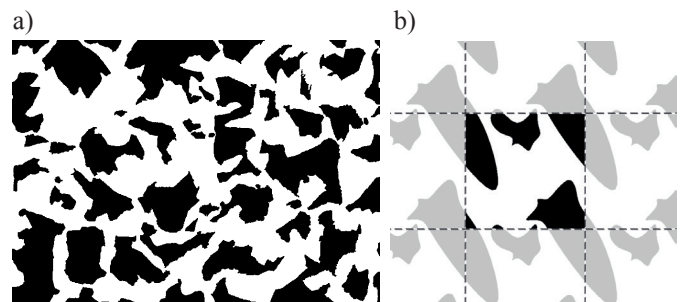


Fig. 1. Idea of the SSRVE – a) micrograph after binarization representing RVE, b) statistically similar element

### 2.2 Construction of the SSRVE for two-phase steels

Basic principles of the construction of the SSRVE and examples of calculations for selected microstructures are presented briefly in this chapter, see [9] for details. The process of SSRVE creation consists of the steps presented in figure 2 including: image analysis, reconstruction of 3D microstructure, extraction and selection of shape coefficients, construction of a cost function for optimization procedures, implementation of a proper optimization method and selection of the best result. The reliability of SSRVE depends on all of the steps, but the most influential element is the optimization procedure, where genetic algorithm (GA) is applied. The representation of the specimen in this algorithm is based on Non-Uniform Rational B-Splines (NURBS) control points, which are used to represent SSRVE in each iteration. The applied

objective function compares reference coefficients of a real microstructure with SSRVE coefficients calculated for current NURBS representation.

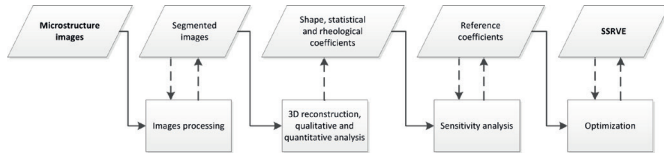


Fig. 2. Diagram of SSRVE creation

Particular steps enumerated above are characterized by different computational complexity and algorithmic approach. Some of them can be easily parallelized or distributed, which increases computational efficiency of the whole approach. In the case of image analysis, coefficients calculations, sensitivity analysis (SA) and optimization, most of the computational operations can be performed separately without necessity of synchronization. These steps were selected for the purpose of parallelization and will be described in details in further sections.

### 2.2.1 Image analysis

The main steps of the image analysis are filtering, segmentation and reconstruction, which takes place in the case of 3D analysis. Filtering is based on the Dynamic Particles algorithm, which was designed as an approach for denoising of data with different dimensionality including 1D plot, 2D images and  $n$ D measurements. The details of this method can be found in [12]. The filtering removes high frequency noise from the input images allowing to strengthen visibility of boundaries between phases and grains. Afterwards the segmentation stage is applied consisting of two steps, i.e. separation of phases and detailed analysis of grains inside each phase. The typical values of thresholds, which separates the light and dark phases on the image, usually cover the first minimum or the first inflexion point located on the histogram on the left side of the peak. They were determined and described in details in [13]. This enabled application of the boundary detection algorithms and separation of different grains within each phase. Example of results obtained for typical DP steel, where fraction of martensite is lower than 30%, are presented in figure 3.

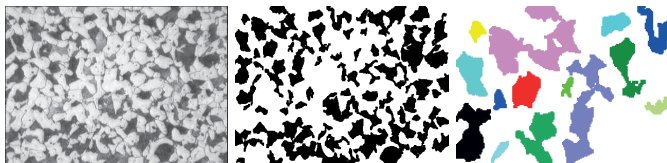


Fig. 3. Results of image segmentation, (a) original DP image, (b) divided phases, (c) separated grains

The microstructure images uploaded as an input to the procedure of SSRVE creation can be analysed separately in  $n$  different computing threads without synchronization. This

allows to obtain high speedup and scalability, which results in reduction of time spend on filtering ( $t_f$ ) and segmentation ( $t_s$ ) of  $n_i$  images:  $t_{fs} = \max(t_f + t_s)$ . However, the last stage of the image analysis, i.e. reconstruction, is usually performed sequentially. The results obtained from segmentation and labelling are passed in proper sequence to reconstruction procedure, which merges particular 2D grains into 3D objects. The reconstruction is hardly distributed agglomerative procedure, which requires synchronization of crucial reconstruction steps. It should be distributed as  $n_i/2$  computing threads. Thus, the time required for full reconstruction can be reduced from  $t_r = n_i \cdot t_m$  down to  $t_r = \log_2(n_i) \cdot t_m$ , where  $t_m$  is an average merging time for two subsequent images. Theoretically, the final time of image processing of  $n$  microstructure images is:

$$t_{ip} = \max(t_f + t_s) + \log_2(n_i) \cdot t_m \quad (1)$$

### 2.2.2 Shape coefficients

The set of segmented images or reconstructed 3D microstructure is passed to further analysis based on the shape coefficients calculations, which are performed for all grains. Shape coefficients were the main factors, which were used in [9] to design the optimal shape of the SSRVE. Usually thirteen shape coefficients are considered. Nine of them describe geometrical shape of analysed object in 2D and 3D domain. These are: volume fraction, interfacial surface to volume ratio, dimensionless interfacial surface to volume ratio, roundness, ellipsoid fit, ratio between the minimum and maximum distance between contour and the centre of the martensite island, border index, curvature of the surface and specific integral of the total curvature. Remaining four coefficients are dedicated to processing of digital images. These are: Malinowska, Blair-Bliss, Danielsson, Haralick.

Two-level hierarchical parallelization of shape coefficients calculations can be applied. The higher level parallelization distribute grains to computing hardware infrastructure as  $n_g$  different computing jobs, where  $n_g$  is a number of grains. In the lower level parallelization each of  $k$  shape coefficients are calculated in  $k$  separated threads. Theoretically, this allows to reduce the time of shape coefficients calculations to:

$$t_{sc} = \max(t_k) \quad (2)$$

where  $t_k$  is time required to calculate single shape coefficient for one grain.

### 2.2.3 Sensitivity analysis and optimization

Numerical tests performed by the Authors of this paper have shown that using only shape criteria in designing the SSRVE may cause problems with the uniqueness of the solution. It was observed that the influence of the shape of inclusion, as well as its location and twisting, on stress and strain distribution, is also important. The deeper analysis showed that it is not trivial problem to find the relation between the shape of the inclusion and stress/strain distributions. Therefore, the information on

strain and stress has to be a part of the procedure of SSRVE creation, where SA and optimization take place. The calculations of SA as well as optimization procedure are based on the same objective function, which, in the case of SA, is used to determine the influence of input parameters on its value and, in the case of optimization, is used to find the best shape of SSRVE. Therefore, the definition of the objective function is crucial for further investigation. It is given by the equation composed of three internal elements responsible for identification of shape coefficients, statistical measures and rheological behaviour:

$$\Phi = \sqrt{\sum_{i=1}^k w_i \zeta_i^2 + \sum_{i=k+1}^{k+l} w_i \varphi_i^2 + \sum_{s=1}^3 \left( w_s \sum_{j=1}^p \sigma_{sj}^2(\varepsilon_j) \right)} \quad (3)$$

where  $\zeta_i = \frac{\zeta_{iRef} - \zeta_{iSSRVE}}{\zeta_{iRef}}$  is a comparison of  $i$ -th shape

coefficient,  $\varphi_i = \frac{\varphi_{iRef} - \varphi_{iSSRVE}}{\varphi_{iRef}}$  is a comparison of statistical

measures and  $\sigma_{sj} = \frac{\sigma_{sjRef} - \sigma_{sjSSRVE}}{\sigma_{sjRef}}$  is a comparison of

stresses obtained for three different deformations of referential microstructure and SSRVE, i.e. compression, tensile and shear,  $w_i$  are optimization weights,  $k$  – number of shape coefficients,  $l$  – number of statistical measures,  $s$  – number of rheological curves,  $p$  – number of iterations in numerical simulations. Such approach allows to compare not only individual numbers but the whole rheological curves identified for microstructure and SSRVE, where  $\varepsilon_j = \frac{1}{S} \int \varepsilon ds$  and  $\sigma_{sj} = \frac{1}{S} \int \sigma ds$  are calculated in each iteration of numerical simulation ( $S$  is the area of the microstructure or SSRVE sample).

The critical issue in the design of the best optimization function is estimation of proper weights  $w_i$  for each element under the square root. Such information can be obtained by using SA, which, according to results from initial investigation [9], has to be applied individually for each microstructure. Three different microstructures were analysed in [9], but only Malinowska coefficient had similar values and distributions in all the cases. The remaining problems encountered in [9] were as follows:

- The analysed shape coefficients did not return reliable results for large grains with sophisticated shapes and enclosed background phase.
- Number of elements inside the SSRVE influenced the value of the cost function.
- The procedures calculating perimeter and area of an analysed object does not take into account real shape of an object but its digitalized approximation, what may lead to negative values of the coefficient.

Both procedures, i.e. sensitivity analysis and optimization, use numerically intensive simulations enclosed in common objective function. Therefore, to increase computational performance they can be parallelized or distributed. The calculations in SA are usually based on previously executed “SA method-dependent” space

sampling, which generates values of input data used by objective function. Due to such pre-sampling, the objective function can be evaluated separately for each data and no partial synchronization is required. The time of SA is reduced to  $t_{SA} = \max(t_{of})$ , where  $t_{of}$  is time spent on evaluation of objective function. The obtained results are passed to SA function, which analyses input-output dependencies. During an execution of the optimization procedure, based on GA, each of the specimen in the population can be evaluated separately. Thus, the time of optimization is dependent mainly on the number of iterations  $n_{it}$ :  $t_{opt} = n_{it} \cdot \max(t_{q-ob})$ , where  $t_{q-ob}$  is the time spent on evaluation of the objective function in  $q$ -th iteration of optimization.

### 3. Strategy of parallelization and distribution

The theoretical time required for full procedure of SSRVE creation is composed of times spent on subsequent procedures of image analysis, estimation of shape coefficients, sensitivity analysis and optimization:

$$t_{SSRVE} = \max(t_f + t_s) + \log_2(n_i) \cdot t_m + \max(t_k) + \max(t_{of}) + n_{it} \cdot \max(t_{q-ob}) \quad (4)$$

where  $t_f$  – filtering time,  $t_s$  – segmentation time,  $t_m$  – an average merging time of two subsequent images,  $n_i$  – number of microstructure images,  $t_k$  – time required to calculate single shape coefficient for one grain,  $t_{of}$  – time spent on evaluation of objective function,  $n_{it}$  – number of iterations and  $t_{q-ob}$  – time spent on evaluation of the objective function in  $q$ -th iteration of optimization. It is just theoretical estimation based on assumption that hardware resources are unlimited. In real life calculations, such solution cannot be achieved, mainly because of large number of samples required by sensitivity analysis. Thus, the following correction in the equation should be introduced:

$$t_{SSRVE} = \max(t_f + t_s) + \log_2(n_i) \cdot t_m + \max(t_k) + \frac{N}{n_i} \cdot \max(t_{of}) + n_{it} \cdot \max(t_{q-ob}) \quad (5)$$

where  $N$  is number of samples and  $n_i$  is a number of threads running concurrently on hardware infrastructure. The rest of the calculations should be performed with the assumption that:

$$t_{SSRVE} = \max(t_f + t_s) + \log_2(n_i) \cdot t_m + \max(t_k) + \frac{N}{n_i} \cdot \max(t_{of}) + n_{it} \cdot \max(t_{q-ob}) \quad (6)$$

where  $n_i$  – number of microstructure images,  $n_g$  – number of all grains,  $k$  – number of coefficients,  $n_{pop}$  – number of specimens in GA population. The main challenge, besides the actual implementation of SSRVE procedure, is to develop a custom code to coordinate the infrastructure-related part of calculations, i.e. authorization, scheduling of computing jobs to workers, monitoring of progress and gathering results. This custom code has to be fault-tolerant to guarantee that the process will finish in the case of various failures. Scalarm platform [14], which facilitates so called data farming computing is used in for this purpose in the

paper. It integrates with different hardware infrastructures including the PL-Grid, Amazon EC2 and private ssh-accessible servers to execute numerical procedures passed to Scalarm in form of binaries. The most important benefit of applying Scalarm to SSRVE creation is a complete elimination of the coordination code from the SSRVE-related side. Moreover, the user is provided with Graphical User Interface (GUI), presented in figure 4, for management of computing jobs and progress monitoring of computations without any additional effort.

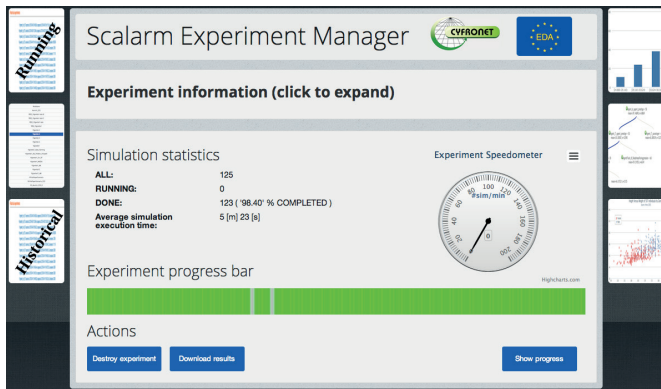


Fig. 4. The progress monitoring view of an experiment in Scalarm

To conduct the parameter study with Scalarm, the user had to provide: actual binaries for generating SSRVE, a description of the generation process input, and an adapter to transform input parameters for the binaries from the Scalarm-native format to the SSRVE-native format. The actual binaries for SSRVE creation are not modified due to the adapter pattern applied to preparation of the input parameters and translation of the output. The workflow of computing jobs is related to diagram presented in figure 2.

#### 4. Results

The numerical calculations were performed for two-phase steel with hard phase volume fraction equal to 45%. Selected picture of the image analysis for this steel, which was used in calculations of shape coefficients, is shown in figure 5.

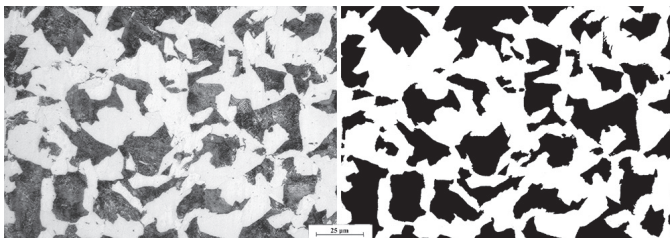


Fig. 5. Part of two-phase steel microstructure with 45% of martensite: original micrograph (a), binarized image (b)

The size (width and height) of SSRVE elements was calculated according to RVE size (575 $\mu$ m width x 405 $\mu$ m height) and for assumed phase fraction. SA performed for

various shape coefficients for the investigated microstructure allowed to determine three referential coefficients, which were selected for further optimization:

- Malinowska coefficient

$$\left(\zeta_1 = \frac{L_m}{2\sqrt{\pi S_m}} - 1\right), \zeta_{1\_REF} = 0.572$$

- LP2 coefficient ( $\zeta_2 = \frac{L_m}{L_{m_{max}}}$ ),  $\zeta_2 = 0.92$

- maximum curvature

$$\left(\zeta_3 = \frac{1}{2V_m} \int \left( \min_{\beta}[\kappa] + \min_{\beta}[\kappa] \right) dS_m \right), \zeta_3 = 4.96$$

where:  $S_m$ ,  $L_m$  – an area and a perimeter of an analysed object,  $\beta$ – the direction in the tangential plane,  $\kappa = \kappa(\beta)$ – curvature. The initial microstructure was deformed by compression, tension and shearing to obtain reference flow curves. The results of optimization for selected material is presented in figure 6a The comparison of three flow curves, being the part of the objective function, are shown in figure 6b. Figure 7 presents comparison of stress distribution in microstructure and SSRVE obtained in compression test.

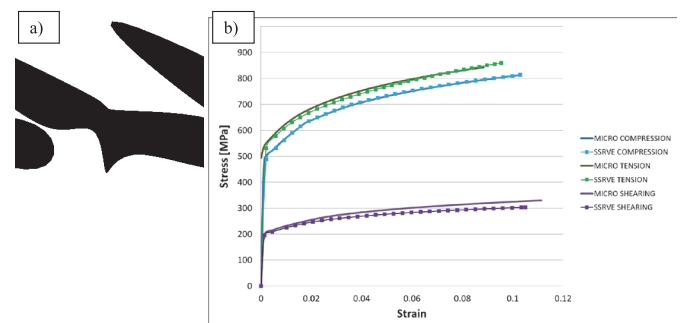


Fig. 6. Obtained SSRVE (a) and comparison of flow curves between microstructure and SSRVE obtained for compression, tension and shearing (b)

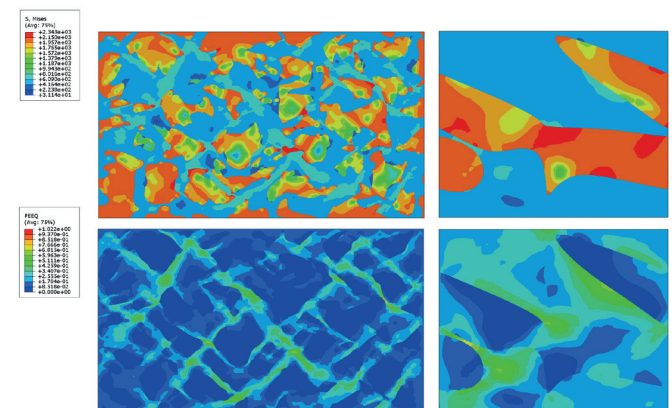


Fig. 7. Effective stress [MPa] distribution after compression of microstructure and SSRVE with 10% reduction

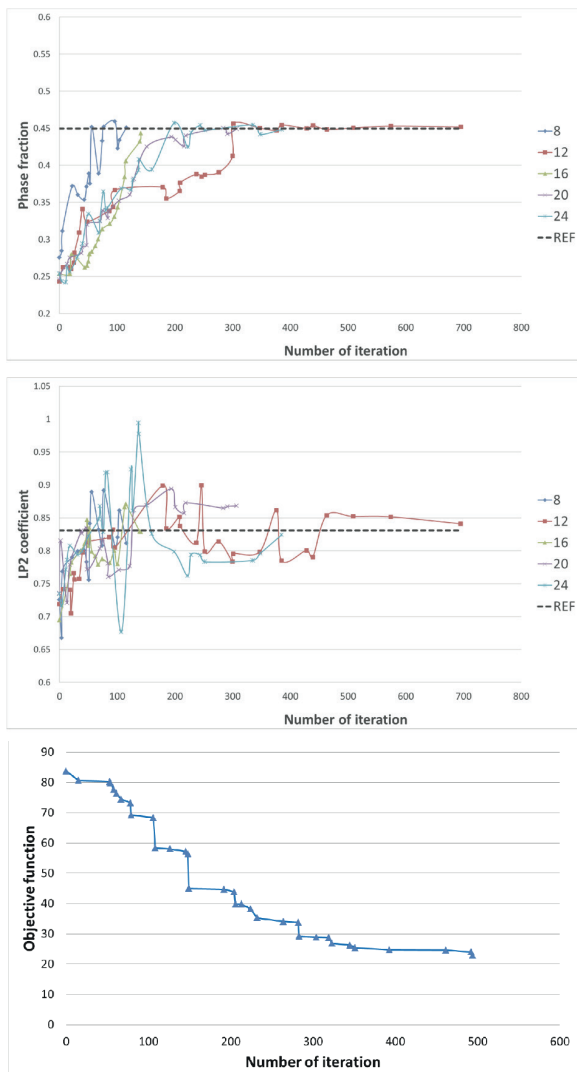


Fig. 8. Convergence of optimization procedure for two coefficients (for different number of NURBS control points) and objective function (12 NURBS control points)

The optimization procedure was tested for 3<sup>rd</sup> degree NURBS with different number of control points (8, 12, 16, 20 and 24), which are used to create reliable representation of SSRVE. The best result was obtained for 12 control points after 350 iterations, which took about 260 hours in sequential mode (not parallelized and not distributed) executed on Intel i5 2500K. This time includes: data preparation (image analysis of microstructure, calculation of shape coefficients and deformation), The most demanding part of optimization are numerical simulations of compression, tension and shearing, which take 19s, 17s and 29s respectively. The whole procedure was improved by distribution and parallelization described in previous chapters, which reduced computing time to about 8 hours by using 40 computing nodes. Such approach allowed to parallelize estimation of objective function in all specimens of optimization algorithm. Synchronization of results was applied after each iteration of optimization.

## 5. Conclusions

The paper presents approach to creation of the SSRVE, where conventional objective function, based on shape coefficients and phase fraction, was modified with component accounting for strain and stress values in the SSRVE under loading conditions. The introduction of these two components was justified by observations that shape, location and torsion of inclusion in the SSRVE influences strain and stress distributions. The relation between characteristics of inclusions and calculated distribution is not trivial, thus the introduction of new components into objective function cannot replace the previous ones determining the shape coefficients. The obtained results proved that behaviour of deformed material is much better reflected by SSRVE created with new objective function. This allows to replace sophisticated representation of material microstructure (total number of nodes: 30584, total number of linear triangular elements: 60675) by simplified computing domain of SSRVE (total number of nodes: 2725, total number of linear triangular elements: 5246), while no loss of quality is observed. Therefore, the time spent on creation of SSRVE will be retrieved during application of SSRVE in multiscale numerical simulations.

Recent investigation shown that computing domain of SSRVE can be further reduced by replacement of finite element method by Isogeometric Analysis (IGA). This approach is originally based on NURBS representation of geometry, which is convergent with native representation of SSRVE. Development of IGA based approach will be the main direction of the future work.

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