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TWO-STEP HOMOGENIZATION OF ASPHALT MIXTURES

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Summary: *A novel approach to the prediction of nonlinear macroscopic response of asphalt mixtures is presented. It combines well established first order homogenization method and a concept of so called statistically equivalent periodic unit cell. Such a unit cell allows us to take into account a real microstructure of asphalt mixture when searching for the estimates of nonlinear macroscopic response. To that end, both the finite element and the Fast Fourier Transform methods are examined. Several numerical examples are presented to show applicability of the proposed approach.*

1. Introduction

The main objective of this contribution is to provide estimates of the effective properties of asphalt mixtures shown in Fig. 1a. Computational analysis taking into account all geometrical details of a two-phase microstructure (stone aggregates bonded to a bitumen matrix) would, however, be prohibitively expensive. The search for an efficient computational scheme is therefore needed.

The proposed approach relies on a popular uncoupled multi-scale homogenization technique taking advantage of the concept of statistically equivalent periodic unit cell. To arrive at the desired effective properties requires completing the following steps:

- Preparing a binary image of a real microstructure. This step leads to a set of representatives of the real microstructure with variable volume fraction of stone aggregates generated by gradually removing stones up to a given size from the original microstructure. While removing small stones simplifies the microstructure complexity on the one hand, it reduces the overall stiffness on the other hand. Substituting the actual matrix with a homogenized equivalent medium based on the volume of removed stones appears therefore inevitable leading to a two-scale uncoupled homogenization. This step, however, goes beyond the present scope and will not be addressed herein. Instead, the interesting reader is referred to (Valenta & Šejnoha, 2007).
- Formulation of a statistically equivalent periodic unit cell (SEPUC) by comparing the material statistics, e.g. the two point probability function, of the most appropriate representative of the real microstructure and the periodic unit cell as suggested in

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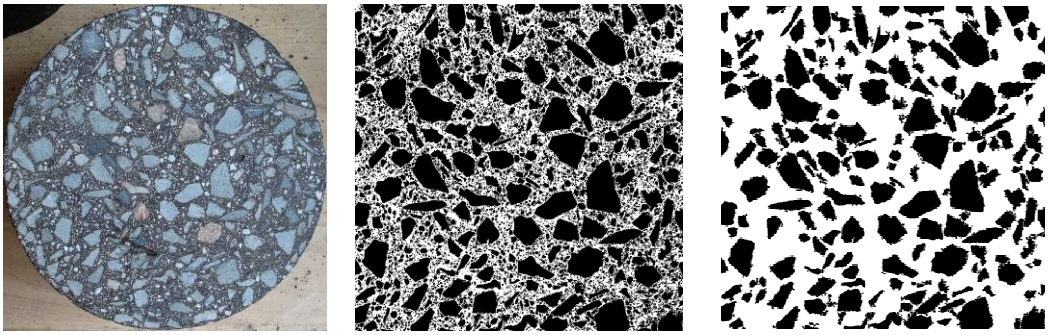
(Zeman & Šejnoha, 2001), (Zeman & Šejnoha, 2007). Section 2 summarizes the most important steps of this topic.

- Evaluation of the non-linear effective properties for the periodic unit cell. This topic including a description of the nonlinear viscoelastic material model is discussed in Section 3 and 4.



(a) (b) (c)

Fig. 1: (a) A real microstructure of an asphalt mixture, (b) A binary image of an RVE taken from the original color image, (c) A binary image after eliminating stone fragments smaller than (in area) 1200 pixels 4.97 mm^2

2. Formulation of SEPUC

Although considerable savings in computational time can be achieved with coarse RVEs, the analysis employing original microstructures still presents a significant challenge particularly in view of a large scale nonlinear analysis of multi-layered rodes. A possible route that further contributes to the efficiency of the computational analysis is discussed here in conjunction with a statistically equivalent periodic unit cell (Zeman & Šejnoha, 2001).

Suppose that the original microstructure can be replaced by a certain artificial periodic unit cell that, from the microstructure point of view, statistically resembles the real material system in terms of, e.g. the two-point probability function. Such a unit cell can be defined by the following parameters: number of aggregates having elliptical shape, size, position, orientation and aspect ratio of the axes of individual ellipses. The size of stones is derived based on the cumulative distribution function (Valenta & Šejnoha, 2007). For example, if 10 stones are selected for a PUC then the smallest stone corresponds to an average size of 10% of the smallest stones determined from the cumulative distribution function. The next stone then reflects the size of the subsequent 10% stones, etc. Examples of such unit cells are depicted in Fig. 2, which correspond to modified real microstructure depicted in Fig. 1c.

The key step in the definition of the optimal periodic unit cell is a choice of the proper description of heterogeneous materials with a random structure. In the present work, we limit our attention to two specific descriptors – the one- and two-point probability functions S_r and S_{rs}, see e.g. (Torquato, 2005) for more details and examples of alternative statistical descriptors. The statistically optimal values of PUC parameters (in case of 10 ellipses the geometry is determined by forty parameters) then follow from minimization of the least square error

$$E = \sum_i \sum_j \left(S_{rs}^0(i, j) - S_{rs}(i, j) \right)^2, \tag{1}$$

where S_{rs}^0 is the two-point probability function related to the original microstructure while S_{rs} stands for the two-point probability function of the idealized unit cell.

A closer inspection reveals that the objective function E is non-convex, multimodal and discontinuous due to the effect of limited bitmap resolution. Based on previous works (Hrstka & Kučerová & Lepš & Zeman, 2003), (Matouš & Lepš & Zeman & Šejnoha, 2000), a global stochastic optimization algorithm that relies on the combination of real-valued genetic algorithms and the simulated annealing method is employed to solve this optimization problem.

The algorithm used for the optimization of the objective function S_{rs} is based on an evolutionary algorithm GRADE (Hrstka & Kučerová & Lepš & Zeman, 2003). The first step in the algorithm is to generate a starting generation of possible periodic unit cells by choosing random values of all state variables. The size of the population (the number of PUCs to be simultaneously modified during minimization process) is in our case set to 100. After the initiation stage the following steps are repeated within each iteration until a termination condition is reached:

1. MUTATION, which creates a new solution **x** using the operation

$$\mathbf{x} = \mathbf{y} + k(\mathbf{y} - \mathbf{z}), \tag{2}$$

   where **y** is a solution from actual population, **z** is a randomly created solution and *k* is a real number from given bounds. Thirty percents of solutions in a new population are created by this operator.

2. CROSS-OVER, which creates a new solution **x** according to

$$\mathbf{x} = opt(\mathbf{y}, \mathbf{z}) + cs(\mathbf{y} - \mathbf{z}), \tag{3}$$

   where **y** is a solution from actual population, **z** is a randomly created solution and *k* is a real number from given bounds. Thirty percents of solutions in a new population are created by this operator.

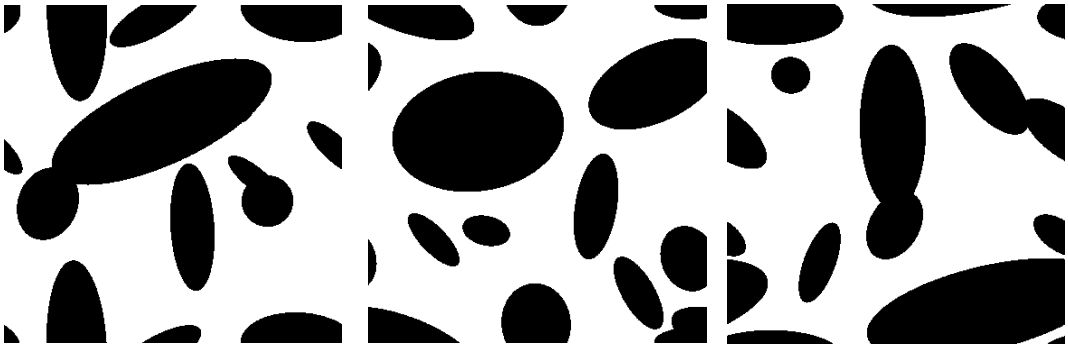
3. EVALUATION computes the objective function value for each new solution.

4. TOURNAMENT SELECTION, where the worst individual from two randomly selected solutions is deleted. This operator is repeated until the number of solution is the same as at the beginning of the cycle.

The basic version of GRADE is complemented with CERAF strategy (Hrstka & Kučerová, 2004) in order to increase the algorithm robustness when dealing with multi-modal problems. The CERAF strategy works on the principle of multi-start. If the best value found by a stochastic algorithm does not change for more than a prescribed value during a certain number of generations, CERAF stores the optimal point in memory and surrounds it by a "radioactive" zone defined as *n*-dimensional ellipsoid with each diameter equal to 25% of the size of searched domain. If a new solution is located inside the "radioactive" zone, it is

replaced with a random one outside the zone. This should prevent a premature convergence to a local minimum. For more details see (Hrstka & Kučerová, 2004).

As typical of genetic algorithms-based optimization problems a single run yields one particular unit cell. Running the optimization problem again with a new starting population usually provides a unit cell with the same statistics but slightly different geometrical details. Three examples of the statistically optimal PUCs derived from three consecutive runs are shown in Fig. 2. It remains to show that these unit cells provide more or less identical macroscopic elastic homogenized properties (Valenta & Šejnoha, 2008).



a) SEPUC 43 b) SEPUC 37 c) SEPUC 6

Figure 2: Examples of SUPUC corresponding to binary image after eliminating stone fragments smaller than 1200 pixels

3. Local constitutive law

In the numerical model two phases of asphalt mixtures are considered – stone phase and mastic phase. Mastic asphalt is a composite consisting of a bitumen matrix and a very fine stone fraction. In accord with (Read & Whiteoak, 2003) the bitumens are non-linear viscoelastic materials and their behavior varies from purely non-linearly viscous to wholly elastic depending upon loading time, load level and temperature. Unlike the viscoelastic matrix, the aggregate are expected to follow the linear elastic law.

Here, the generalized Leonov model is assumed to represent the non-linear viscoelastic effects developed in the matrix phase. Combing the Eyring flow model for the plastic component of the shear strain rate

$$\frac{\mathrm{d}e_p}{\mathrm{d}t} = \frac{1}{2A}\sinh\frac{t}{t_0}, \tag{4}$$

with the elastic shear strain rate $\mathrm{d}e_e/\mathrm{d}t$ yields the one-dimensional Leonov constitutive model (Leonov, 1976)

$$\frac{\mathrm{d}e_p}{\mathrm{d}t} = \frac{\mathrm{d}e_e}{\mathrm{d}t} + \frac{\mathrm{d}e_p}{\mathrm{d}t} = \frac{\mathrm{d}e_e}{\mathrm{d}t} + \frac{t}{h\left(\mathrm{d}e_p/\mathrm{d}t\right)}, \tag{5}$$

where the shear-dependent viscosity h is provided by

$$h\left(\mathrm{d}e_p/\mathrm{d}t\right)=\frac{h_0\,t}{t\,\sinh\left(t/t_0\right)}=h_0\,a_s\left(t\right). \tag{6}$$

In (4), A and t_0 are material parameters; a_s that appears in (6) is the stress shift function with respect to the zero shear viscosity h_0 (viscosity corresponding to an elastic response). Clearly, the phenomenological representation of (5) is the Maxwell model with the variable viscosity h .

To describe multi-dimensional behavior of the material, the generalized compressible Leonov model, equivalent to the generalized Maxwell chain model, can be used (Tervoort, 1996). The viscosity term corresponding to the m-th unit receives the form

$$h_m=h_{0,m}\,a_s\left(t_{eq}\right), \tag{7}$$

where the equivalent shear stress t_{eq} is provided by

$$t_{eq}=\sqrt{\tfrac{1}{2}s_{ij}\,s_{ij}}\,, \tag{8}$$

and s_{ij} is the stress deviator tensor. Admitting only small strains and isotropic material, a set of constitutive equations defining the generalized compressible Leonov model can be written as

$$s_m=K\,e_v, \tag{9}$$

$$\frac{\mathrm{d}s}{\mathrm{d}t}=\sum_{m=1}^{M}2G_m\left(\frac{\mathrm{d}e}{\mathrm{d}t}+\frac{\mathrm{d}e_{p,m}}{\mathrm{d}t}\right), \tag{10}$$

$$s_m=2h_m\frac{\mathrm{d}e_{p,m}}{\mathrm{d}t}=2h_m\,a_s\left(t_{eq}\right)\frac{\mathrm{d}e_{p,m}}{\mathrm{d}t}, \tag{11}$$

$$s=\sum_{m=1}^{M}s_m, \tag{12}$$

where s_m is the mean stress, e_v is the volumetric strain, K is the bulk modulus and G_m is the shear modulus of m-th unit. A possible approach to the numerical solution of the differential equation (10) is shown i.g. in (Valenta & Šejnoha, 2008).

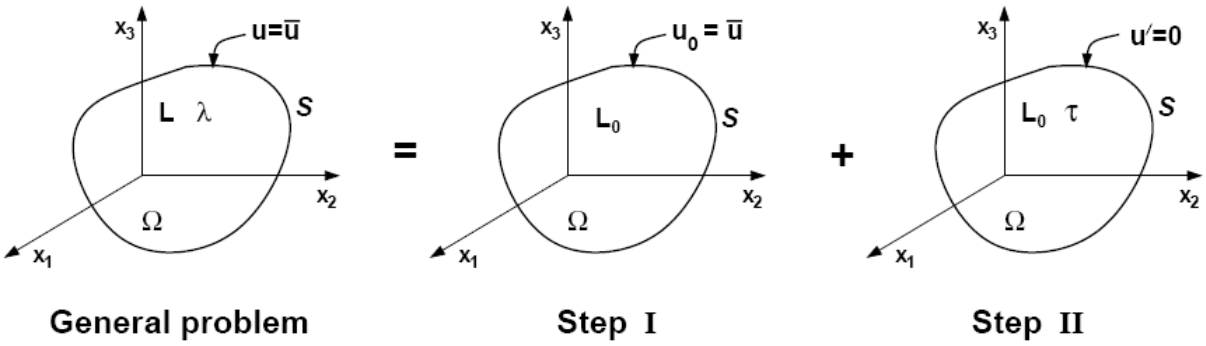


Fig. 3: Body with prescribed surface displacements including eigenstresses

4. Microscale modeling via FFT-based method

An iterative numerical method based on fast Fourier transform (FFT) has been proposed by Moulinec and Suquet (Michel & Moulinec & Suquet, 1999) to investigate the effective properties of composites with complex microstructures as well as their local response. The method is based on the exact expression of the Green function for a linear elastic, homogeneous material.

The macroscopic non-linear viscoelastic response of RVE is obtained through the solution of the local problem, which consists of the equilibrium and constitutive equations complemented by boundary conditions. With reference to the general problem displayed in Fig. 3 we consider an anisotropic and heterogeneous body loaded by an affine displacement field $\boldsymbol{u}_0(\mathbf{x}) = \boldsymbol{E} \cdot \mathbf{x}$. The local constitutive law including incremental eigenstresses $\Delta\lambda$ then reads

$$\begin{aligned} \Delta\boldsymbol{\sigma}(\mathbf{x}) &= \mathbf{L}(\mathbf{x}) : \Delta\boldsymbol{\varepsilon}(\mathbf{x}) + \Delta\lambda(\mathbf{x}) \quad \text{in } \Omega \\ \mathbf{u} &= \overline{\mathbf{u}} \quad \text{in S.} \end{aligned} \tag{13}$$

As suggested by Hashin-Shtrikman (Hashin & Shtrikman, 1962) the local stress and strain fields in (13) can be found from the two auxiliary boundary value problems, Fig 3. The procedure starts by assuming a geometrically identical body with a certain reference homogeneous, but generally anisotropic, medium $\mathbf{L}_0$ and same prescribed displacements. The corresponding incremental uniform strain $\Delta\boldsymbol{E}$ and stress $\Delta\boldsymbol{\Sigma}$ fields are related through a constitutive law in the form

$$\Delta\boldsymbol{\Sigma} = \mathbf{L}_0 : \Delta\boldsymbol{E} \quad \text{in } \Omega; \quad \mathbf{u}_0 = \overline{\mathbf{u}} \quad \text{in S.} \tag{14}$$

Following the Hashin-Shtrikman idea, we introduce the increment of the symmetric stress polarization tensor $\Delta\boldsymbol{\tau}$ such that

$$\Delta\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{L}_0(\mathbf{x}) : \Delta\boldsymbol{\varepsilon}(\mathbf{x}) + \Delta\boldsymbol{\tau}(\mathbf{x}). \tag{15}$$

The periodic boundary conditions are expressed as a decomposition of strain increments into an average $\Delta\boldsymbol{E}$ and a fluctuating part $\Delta\boldsymbol{\varepsilon}^*(\mathbf{x})$ over the RVE

$$\Delta\boldsymbol{\varepsilon}(\mathbf{x}) = \Delta\boldsymbol{E} + \Delta\boldsymbol{\varepsilon}^*(\mathbf{x}). \tag{16}$$

It is clear, that the increment of stress polarization tensor is given by

$$\Delta\boldsymbol{\tau}(\mathbf{x}) = \left(\mathbf{L}(\mathbf{x}) - \mathbf{L}^0\right) \Delta\boldsymbol{\varepsilon}(\mathbf{x}) - \Delta\lambda(\mathbf{x}). \tag{17}$$

Once the polarization stress is known, the local strain field $\Delta\boldsymbol{\varepsilon}(\mathbf{x})$ can be obtained via Green's function $\boldsymbol{\Gamma}^0$ (an isotropic reference medium was considered in this work) for a given reference medium in the form, see e.g. (Zeman & Šejnoha, 2007),

$$\Delta\boldsymbol{\varepsilon}(\mathbf{x}) = \Delta\boldsymbol{E} - \int_\Omega \boldsymbol{\Gamma}^0(\mathbf{x} - \mathbf{x}') \, \Delta\boldsymbol{\tau}(\mathbf{x}') \mathrm{d}\mathbf{x}' . \tag{18}$$

After inserting the polarization stress $\Delta\boldsymbol{\tau}$ into (18) we obtain the so called *periodic Lippmann Schwinger* integral equation for a given reference medium as

$$\Delta\boldsymbol{\varepsilon}(\mathbf{x}) + \int_\Omega \boldsymbol{\Gamma}^0(\mathbf{x} - \mathbf{x}') \left[\left(\mathbf{L}(\mathbf{x}') - \mathbf{L}^0\right) \Delta\boldsymbol{\varepsilon}(\mathbf{x}') - \Delta\lambda(\mathbf{x}) \right] \mathrm{d}\mathbf{x}' = \Delta\boldsymbol{E} . \tag{19}$$

The numerical procedure for solving this equation is based on the fact that the term $\int_{\Omega} \boldsymbol{\Gamma}^0(\mathbf{x}-\mathbf{x}')\,\Delta\boldsymbol{\tau}(\mathbf{x}')\mathrm{d}\mathbf{x}'$ can be efficiently evaluated using Fourier transform techniques as a part of the following algorithm:

0. Initialize: $k=0,\ \Delta\boldsymbol{\varepsilon}^0=\Delta\boldsymbol{E},\ \Delta\boldsymbol{\sigma}^0=\mathbf{L}(\mathbf{x})\Delta\boldsymbol{E}$
1. Compute $\Delta\boldsymbol{\tau}^k(\mathbf{x})=\Delta\boldsymbol{\sigma}^k(\mathbf{x})-\mathbf{L}^0\ \Delta\boldsymbol{\varepsilon}^k(\mathbf{x})$
2. Compute $\Delta\tilde{\boldsymbol{\tau}}^k$ and $\Delta\tilde{\boldsymbol{\sigma}}^k$ by Fourier Transform ($\tilde{\cdot}$ represents the original value in the Fourier space)
3. Convergence test: $err^k \le tol$.
4. Set
   $\Delta\tilde{\boldsymbol{\varepsilon}}^{k+1}(\xi)=-\tilde{\boldsymbol{\Gamma}}^0\ \Delta\tilde{\boldsymbol{\tau}}(\xi)$ for $\xi\neq 0$ Fourier Transform of (25)
   $\Delta\tilde{\boldsymbol{\varepsilon}}^{k+1}(\xi)=\boldsymbol{E}$ for $\xi=0$
5. Compute $\Delta\boldsymbol{\varepsilon}^{k+1}$ by inverse Fourier Transform.
6. Set $\Delta\boldsymbol{\sigma}^{k+1}(\mathbf{x})=\mathbf{L}(\mathbf{x}):\Delta\boldsymbol{\varepsilon}^{k+1}(\mathbf{x})+\Delta\boldsymbol{\lambda}(\mathbf{x})$.
7. $k = k + 1$, go to step 1.

ε_{xy} [-]

Fig. 4: Macroscopic non-linear response from different SEPUC: stress – strain curve

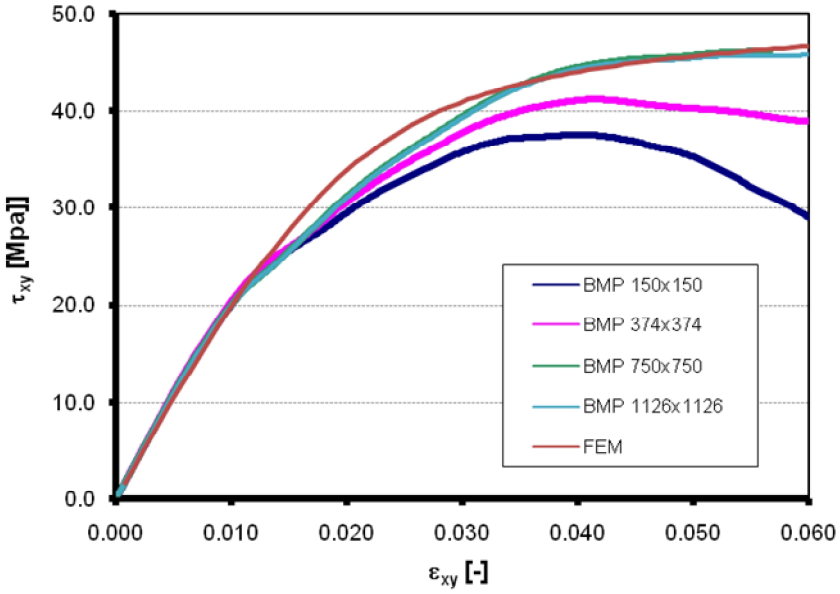


Fig. 5: Macroscopic non-linear response from FFT on original bitmap, FFT on SEPUC an FEM on SEPUC

5. Results

The validation step of the proposed homogenization approach was performed in (Valenta & Šejnoha, 2008) assuming both phases of an asphalt mixture to be linearly elastic. The effective elastic properties of SEPUCs and original bitmaps were compared. Although slightly different in the SEPUC's geometrical details they all provided nearly the same macroscopic response almost identical to the original microstructure. In this work, the applicability of the approach is further tested for the nonlinear viscoelastic behavior.

Since the experimental program for the derivation of non-linear properties of various bitumen asphalts is currently under way, we adopted (noticing a similar elastic behavior) the same non-linear material properties for the generalized Leonov model that we used for the polymeric matrix in (Valenta & Šejnoha, 2007).

As an example we considered a problem of a unit cell loaded by the prescribed constant rate of the macroscopic shear strain. The resulting macroscopic stress-strain curves are plotted in Fig. 4 for SEPUCs from Fig. 2. The results are rather appealing, since any of the cells can be actually used, providing we are not interested in a particular distribution of the local fields within the cell as depicted in Fig. 6 identifying highly strained regions.

Fig. 5 shows results from a comparative study derived using both the FFT and FEM method to simulate the nonlinear viscoelastic response of an optimal periodic unit cell. In particular, the effect of bitmap resolution on the FFT estimates was tested. While the elastic response shows a reasonable agreement the nonlinear response suggest considerable influence of the bitmap resolution on the calculated macroscopic response. A detailed variation of local strains obtained for SEPUC 37 (Fig. 2a) appears in Fig. 6. Evolution of highly localized zones is also the reason for the observed deviations. Evidently, increasing the bitmap resolution brings the FFT estimates closer to the FE predictions. Recall that the formulation based on the

FFT method is local in Fourier space but non-local in the real space. If the local fields are not sufficiently smooth, the stresses in highly strained zones may become excessively high leading to inability of the present Maxwell chain model to accurately represent such behavior (insufficient number chains).

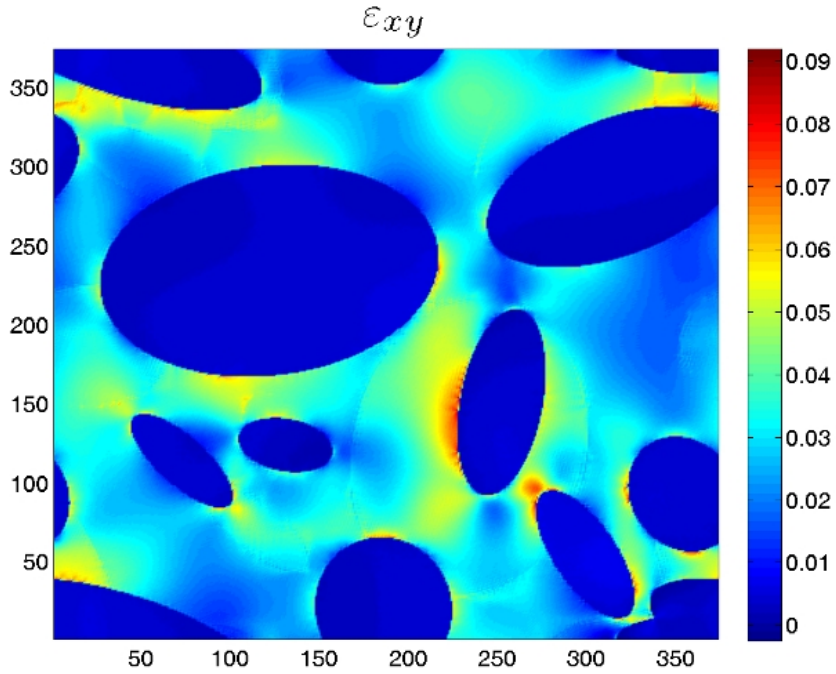


Fig. 6: Variation of local shear strain in SEPUC – overall strain E_{xy} = 0.02

6. Conclusion

This paper summarizes this preliminary work on asphalt mixtures. In our previous works the two-step homogenization procedure was tested assuming a linear elastic behavior of both phases. This contribution extends this strategy to a non-linear behavior of the bitumen matrix. The presented results are rather encouraging. In particular, the FFT method provides results comparable to FE simulations for a properly chosen resolution of the underlying bitmap and therefore be safely applied to actual bitmaps for further validation of the applicability of the derived periodic unit cells. This step together with identification of material parameters of bitumen matrix is, however, still a subject of an ongoing research and will be presented elsewhere.

Acknowledgement

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