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LOCAL HOMOGENIZATION IN MODELING OF HETEROGENEOUS MATERIALS

HOMOGENIZACJA LOKALNA W MODELOWANIU MATERIAŁÓW NIEJEDNORODNYCH

A b s t r a c t

This paper presents the concept of local homogenization method that can be applied to modeling of various heterogeneous materials. Our ultimate goal is to apply it to modeling of asphalt pavement structures and this paper focuses mainly on verification of accuracy and reliability of the method. After a brief characteristic of asphalt properties, the idea of computer homogenization is described. Especially ,the local homogenization is presented in details. Several computational examples (1D and 2D) solved by local homogenization are presented. They are compared with solutions obtained either in analytical way or using directly FEM approach with "full" consideration of heterogeneities in microscale. A few prospective applications of the presented method in context of asphalt pavement structures are depicted.

Keywords: numerical homogenization, heterogeneous media, modeling of asphalt pavement structures

S t r e s z c z e n i e

Artykuł przedstawia koncepcję metody homogenizacji lokalnej, która może być wykorzystana do modelowania różnych materiałów niejednorodnych. Naszym celem jest zastosowanie jej do modelowania konstrukcji nawierzchni asfaltowych, ten artykuł dotyczy głównie sprawdzenia dokładności i wiarygodności metody. Po krótkiej charakterystyce warstw asfaltowych opisano ideę homogenizacji komputerowej. Przedstawiono szczegółowo zwłaszcza homogenizację lokalną. Zaprezentowano kilka przykładów obliczeniowych (1D i 2D) rozwiązanych z wykorzystaniem homogenizacji lokalnej. Wyniki porównano z rozwiązaniami otrzymanymi w sposób analityczny lub poprzez bezpośrednie wykorzystanie MES (z pełnym uwzględnieniem niejednorodności w mikroskali). Przedstawiono kilka perspektywicznych zastosowań prezentowanej metody w kontekście konstrukcji nawierzchni asfaltowych.

Słowa kluczowe: homogenizacja numeryczna, ośrodki niejednorodne, modelowanie konstrukcji nawierzchni asfaltowych

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Denotations

l	–	microscale characteristic dimension
L	–	macroscale characteristic dimension
K, u, f	–	microscale stiffness matrix, degrees of freedom vector, load vector
$\hat{K}, \hat{u}, \hat{f}$	–	macroscale stiffness matrix, degrees of freedom vector, load vector
$X^{\dagger}$	–	Moore–Penrose pseudoinverse of matrix X
$trace(X)$	–	sum of matrix X diagonal elements
$\|X\|^2_{F,B}$	–	Frobenius norm of matrix X weighted with B

1. Introduction

Development of engineering sciences enables us to create new materials with very good characteristics, designed for respective applications. These materials should possess much better features than conventional ones, e.g. stone, wood. They should also provide greater bearing capacity and durability of the structure. Such composite materials are obviously not homogeneous. They consist of several "basic" components, which bound together create a new material possessing much better features than any of the components separately. Due to the complex topology of such composites their direct numerical analysis may be very time consuming. Therefore, a computer homogenization must be used. We intend to use the local homogenization [3, 4] to model asphalt pavement structures which is shown schematically in tab. 1. The paper focuses on verification of this approach by its application to analysis of simple benchmark problems (heat flow and plain strain).

Table 1

Typical asphalt pavement structure (flexible or semi – rigid type)

<table>
<tr><td rowspan="4">Pavement</td><td>Wearing course</td><td>Wearing course</td></tr>
<tr><td>Binder course</td><td>Binder course</td></tr>
<tr><td rowspan="2">Base course</td><td>Roadbase</td></tr>
<tr><td>Subbase</td></tr>
<tr><td colspan="3">Improved subgrade</td></tr>
</table>

In numerical analysis asphalt mix should be treated as visco – elasto – plastic material. Moreover, various asphalt layers (e.g. wearing course vs. binder course) may differ significantly even within the same pavement structure. They usually have different thickness and they are made of different components. That is why, writing "asphalt layer" we don't mean any specific one but this composite type in general.

2. Local homogenization

Let us assume that we analyse an asphalt layer at two separate scales: micro and macro. Both of them are described by respective *characteristic dimensions*. The idea of computer homogenization has already been applied to multiscale modeling of asphalt layers [1]. However, it was done by classical approach based on representative volume elements (RVE) [2]. However, the condition of scale separation has to be satisfied – ratio of micro- (l) and macroscale (L) characteristic dimensions should be much less than 1

$$\frac{l}{L} << 1 \tag{1}$$

It is assumed that the RVE based approach of computer homogenization can be used if above ratio is equal to or less than 0.1. Regarding wearing and binder course, this condition cannot be fulfilled due to their small thickness and respective dimensions of the aggregate. Thus, in paper [1] this approach was applied to asphalt mix represented by one thick layer. Numerical modeling of whole asphalt pavement structure requires a different approach.

The local homogenization method, described in detail in [3], is presented below. In the classical approach FEM mesh is created on the basis of material features in respective subareas. It should consider material discontinuities. In local homogenization we do exactly the opposite. Firstly, the coarse mesh, which covers the whole analyzed region, is generated. Secondly, this mesh is refined inside each element to match the discontinuities. In such a way we create the fine mesh that fully considers material heterogeneities. These two meshes are compatible then. Subsequently, homogenization is done within each element of the coarse mesh. We assess effective stiffness matrices on the basis of fine mesh stiffness matrices. In this approach fulfilment of the condition (1) is not required. Further analysis can be conducted using standard FEM.

Let us focus on fine scale. Let $K \in R^{N\times N}$ be a symmetric stiffness matrix. Local FEM equation can be written as follows

$$Ku = f \tag{2}$$

and $f \in R^N$ is a non – zero load vector. The FEM solution of (2) is equal to

$$u = K^{\dagger} f + u_0 \tag{3}$$

Where $K^{\dagger}$ denotes the Moore–Penrose pseudoinverse of K and u_0 is an arbitrary vector in the null space of K.

Let us consider the same problem in macroscale (coarse mesh). For $M \leq N$ let $\hat{K} \in R^{M\times M}$ be the effective stiffness matrix of coarse element. It is yet unknown.

Load vector in coarse scale is defined as $\hat{f} = A^T f$, where $A \in R^{N\times M}$ is a chosen interpolation operator for a respective element. The FEM coarse – scale solution is equal to

$$\hat{u} = \hat{K}^{\dagger} \hat{f} + \hat{u}_0 \tag{4}$$

Where $\hat{K}^{\dagger}$ denotes the Moore–Penrose pseudoinverse of $\hat{K}$, and $\hat{u}_0$ is an arbitrary vector in the null space of $\hat{K}$. The difference between fine and coarse scale solution is equal then

$$u - A\hat{u} = (K^{\dagger} - A\hat{K}^{\dagger} A^T) f + (u_0 - A\hat{u}_0) \tag{5}$$

Thus, the error $e \in R^N$, up to a constant, is equal to

$$e = (K^\dagger - A\hat{K}^\dagger A^T) f \tag{6}$$

For a non-zero load vector f, known symmetric stiffness matrices for fine mesh elements $K \in R^{N\times N}$, interpolation matrix $A \in R^{N\times M}$, positive – definite symmetric matrix B, dimensionless parameter $\varepsilon > 0$, we look for a symmetric matrix $\hat{K}^\dagger$ that minimizes E, where

$$\mathrm{E}(\hat{K}^\dagger) = \frac{1}{2}\left\|(K^\dagger - A\hat{K}^\dagger A^T) f\right\|_B^2 + \frac{\varepsilon}{2}\left\|K^\dagger - A\hat{K}^\dagger A^T\right\|_{F,B}^2 \left\|f\right\|_2^2 \tag{7}$$

The first term of (7) measures the error of the local solution for a given local load f and is equal to

$$\frac{1}{2}\left\|e\right\|_B^2 = \frac{1}{2} e^T B e \tag{8}$$

The second term is defined as

$$\left\|X\right\|_{F,B}^2 = trace(X^T B X) \tag{9}$$

This is the Frobenius norm “weighted with” B. The second term of (7) is a regularization term and is included to find a unique $\hat{K}^\dagger$. After obtaining matrix $\hat{K}^\dagger$, which minimizes (7), we can find desired matrix $\hat{K}$. Matrix $\hat{K}^\dagger$ is unique and symmetric [3]. Using properties of pseudoinverse matrices we can state that also $\hat{K}$ is symmetric.

A special case of above presented approach is $f = 0$ or is unknown. Expression (7) simplifies then to

$$\mathrm{E}(\hat{K}^\dagger) = \frac{1}{2}\left\|K^\dagger - A\hat{K}^\dagger A^T\right\|_{F,B}^2 \tag{10}$$

Minimization of (10) simplifies significantly the procedure of effective stiffness matrix obtaining. For $B = I$ matrix $\hat{K}$ can be expressed as

$$\hat{K} = \left(A^\dagger K^\dagger (A^\dagger)^T\right)^\dagger \tag{11}$$

3. Examples of local homogenization application

Local homogenization was used to solve below presented examples. Due to a large number of calculations only results with brief descriptions are shown.

3.1. 1D example

Three springs with various spring constants k_i [3]. were connected together as shown below (fig. 1). Only f_1 is assumed to be non-zero. Our task is to find an effective constant k_{eff} of such a connection.

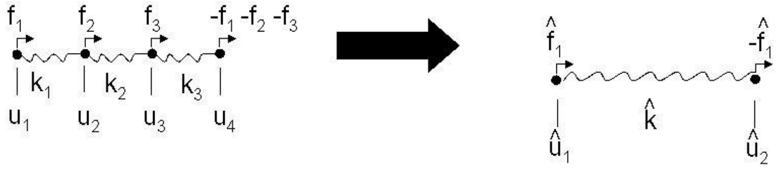

Fig. 1. Three springs connected together "homogenized" as one effective spring

Rys. 1. Homogenizacja trzech połączonych ze sobą sprężyn w jedną sprężynę o efektywnych własnościach

Effective spring constant calculated by means of local homogenization is equal to

$$k^{\mathrm{hom}}_{eff} = \frac{10k_1k_2k_3}{9k_1k_2 + 12k_1k_3 + 9k_2k_3}$$

Whereas analytical solution is equal:

$$k^{analit}_{eff} = \frac{k_1k_2k_3}{k_1k_2 + k_1k_3 + k_2k_3}$$

3.2. 2D example

Heat flow over rectangular shape is analysed in two ways: by means of classic FEM approach, fully considering heterogeneities in microscale and by means of local homogenization using expression (11). By "heterogeneities" we mean 10% of randomly chosen elements with significantly different conductivity constant (k_i = 10 for inclusions, k_m = 1 for the matrix). Inclusions are marked with black in fig. 2. Upper edge of analysed area is heated by flux q = 100 W/m^2, whereas temperature at bottom edge is set as zero. Results of computations are shown in fig. 3.

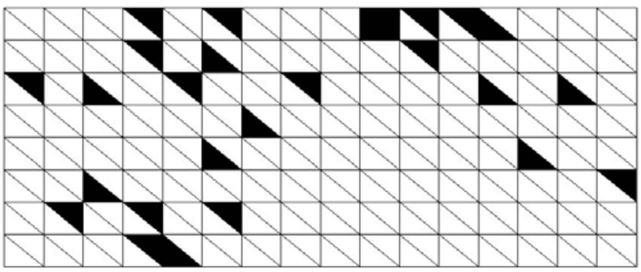

Fig. 2. Matrix and inclusions

Rys. 2. Matryca i inkluzje

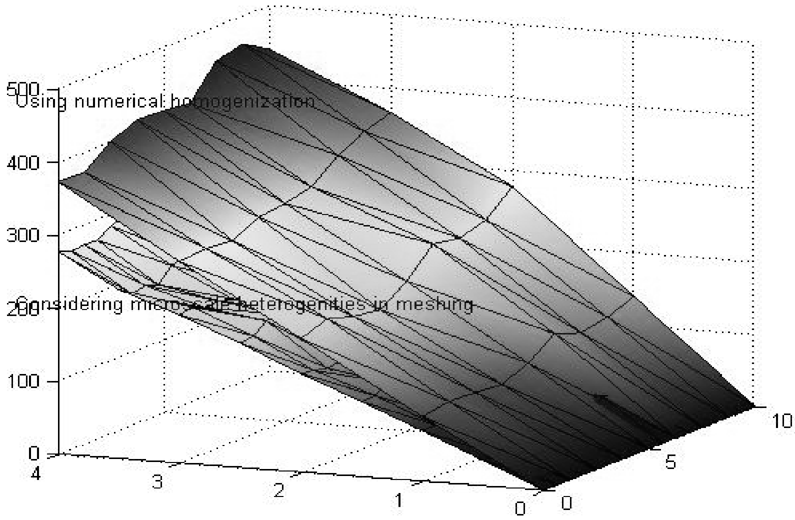

Fig. 3. Temperature within rectangular shape

Rys. 3. Rozkład temperatury wewnątrz prostokątnego obszaru

3.3. 2D example (plain strain state)

This example demonstrates how local homogenization can be applied to modeling of asphalt pavement structure assuming for the sake of simplicity only elastic deformation. A rectangular domain (3,5 m × 1,0 m – dimensions referring to average thickness and width of one road lane) is loaded with wheel. Since the total load is equal to 100 kN/axis, it was divided into two and distributed over respective area reflecting the width of the real tyre. Location of inclusions (aggregate) is shown in fig. 4 ($\nu = 0.3$ for both the matrix and the inclusions, E_1 = 10 GPa for the inclusions and E_2 = 20 GPa for the matrix). We analyse our

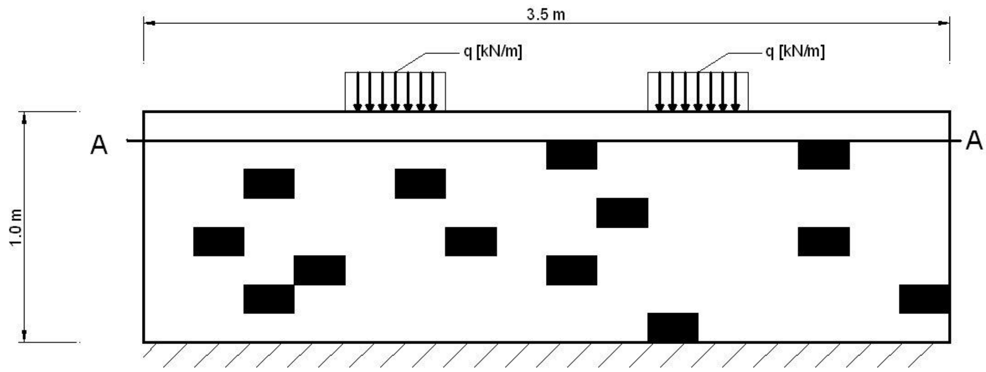

Fig. 4. Scheme of the analyzed domain

Rys. 4. Schemat analizowanego obszaru

problem in two ways. First, it was solved directly by FEM, considering all heterogeneities in microscale. Then it was solved using local homogenization. The plain strain state was assumed for this numerical test purposes. Results – vertical displacements along arbitrarily chosen cross-section A-A (~20 cm under the top of the domain)– are shown in fig. 5. Upper curve was obtained using standard FEM approach (4096 elements), whereas the lower one was obtained using local homogenization (1024 elements). These preliminary results confirm that local homogenization may be a reasonable method of efficient modeling of heterogeneous materials.

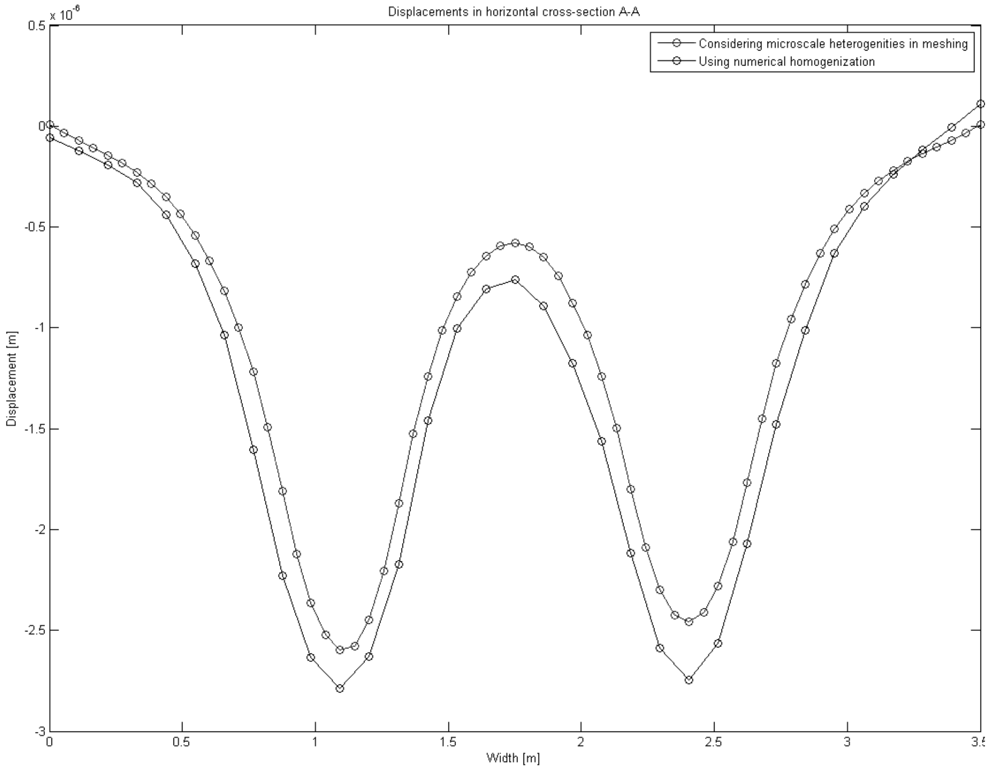

Fig. 5. Vertical displacements along cross-section A-A

Rys. 5. Przemieszczenia pionowe wzdłuż przekroju A-A

4. Conclusions

Concluding our experience with the local homogenisation method we may confirm that this is a promising approach to solution of difficult practical problems. In particular the following aspects should be pointed out:

– separation of scale condition does not have to be satisfied,
– whole pavement structure can be modeled,

– modeling error of the presented solutions is minimum in the sense of the selected norm,
– fast algorithms for computation of pseudoinverses are necessary,
– analysis of the heat flow conducted by application of local homogenization,
– produces solution that significantly differs from the classic one. It is due to the too coarse meshes.

Further analysis will concern modeling of 2D inelastic materials. Then 3D elastic (and subsequently inelastic) materials will be analysed. An experimental validation of the numerical modeling proposed in the paper will be also considered.

References

[1] Dessouki S., *Multiscale approach for modeling hot mix asphalt*, the dissertation, Texas A&M University, College Station 2005.
[2] Kouznetsova V., *Computational homogenization for the multi-scale analysis of multi-phase materials*, the dissertation, TU/e 2002.
[3] Jhurani C.K., *Multiscale Modeling Using Goal-oriented Adaptivity and Numerical Homogenization*, the dissertation, The University of Texas at Austin 2009.
[4] Jhurani C.K., Demkowicz L., *ICES Reports 09-34÷09-36* (http://www.ices.utexas.edu/research/reports/), The University of Texas at Austin 2009.
[5] Strzelecki T., *Mechanika ośrodków niejednorodnych. Teoria homogenizacji*, Dolnośląskie Wydawnictwo Edukacyjne, Wrocław 1996.