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Effective calculation of thermophysical properties of composite materials with multiple configurations by asymptotic homogenization technique

Vasiliy Grigoriev[1], Petr Zakharov[1] and Mir Akimov[2]

[1] International research laboratory "Multiscale model reduction". North-Eastern Federal University, 42 Kulakovskogo st, Yakutsk, 677891, Russian Federation.
[2] Department of Applied Mathematics and Computer Science, North-Eastern Federal University, 48 Kulakovskogo st, Yakutsk, 677891, Russian Federation.

E-mail: d_alighieri@rambler.ru

Abstract. In this work a three-scale asymptotic homogenization technique is considered for calculating the thermophysical properties of composite materials with multiple periodic configurations. Heterogenieties of porous structures were considered by the periodic distribution of single cells at the microscale and mesoscale levels. Two effective thermal conductivity coefficients are calculated to obtain an average solution on the global structure. A three-scale algorithm is also compared with the classical two-scale homogenization, where microscale allows all heterogenieties. We provide a numerical experiments which show the efficiency and accuracy for the calculation of heat transfer of composite material with multiple configurations.

1. Introduction

Porous materials are widely used in engineering and manufacturing because of their good thermal stability, high thermal resistance and low relative density. In particular, in the conditions of the Far North, the issue of thermal insulation is in the first place.

Currently, the materials used in thermal insulation, consist of alternating volumes of substances with different properties. A significant part of such materials are composite materials with a periodic structure.

Averaging methods describe global behaviors by reducing the original equations with fast oscillating coefficients to equations with equivalent coefficients that can not only save computational resources, but also guarantee good computational accuracy [1–9].

In this paper, we thoroughly investigated the process of heat transfer in porous materials with multiple configurations, considered as periodic layers of single cells at the microscale and mesoscale, as illustrated in Figure 1. A level separation approach is used, namely, a three-scale asymptotic homogenization algorithm and comparison of the results obtained with finite element approximation. Also for the interest and completeness of the numerical experiment, the method of classical asymptotic averaging was implemented, where the region is divided into only two scales: micro and macro.

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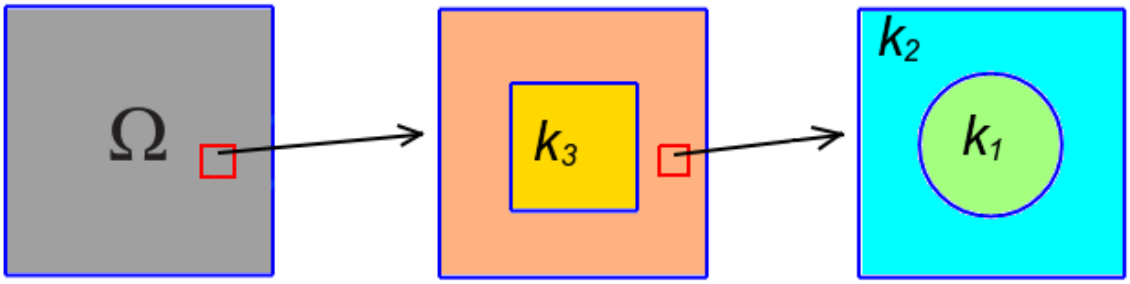

Figure 1. The scheme of the material with multiple configurations. From left to right: macro scale, meso scale, micro scale

2. Three-scale asymptotic homogenization method

In this work, we apply the scale-separation approach, namely a three-scale asymptotic homogenization method, and compare the result with finite element approximation.

Consider the following family of linear elliptic partial differential equations with a periodically oscillating coefficient $a_\varepsilon(x)$ where $\varepsilon \to 0$

$$-\nabla \cdot (a_\varepsilon \nabla u_\varepsilon) = f(x), x \in \Omega \subset \mathbb{R}^2, \tag{1}$$

$$u_\varepsilon(x) = 0, \quad x \in \partial\Omega, \tag{2}$$

where the period of oscillations $a_\varepsilon(x)$ is εL, where L — is domain lenght i.e.,

$$a_\varepsilon(x + k(\varepsilon L)\mathbf{e}_i) = a_\varepsilon(x), \quad \forall k \in \mathbb{Z}, \quad i = \{1, 2\}, \tag{3}$$

where $\mathbf{e}_i$ being the canonical basis $\mathbb{R}^2$. We assume that $f(x)$ is a given function, such that $f \in H^{-1}(\Omega)$.

Now consider the three-scale asymptotic homogenization method. We are considering three different scales, namely d_1, d_2 and L (micro, meso and macro scales), which characterize different structural sizes, i.e.

$$\varepsilon_1 = \frac{d_1}{L} \ll 1 \quad \text{and} \quad \varepsilon_2 = \frac{d_2}{d_1} \ll \varepsilon_1. \tag{4}$$

Using the relation (4) two formally independent variables are introduced:

$$y = \frac{x}{\varepsilon_1} \quad \text{and} \quad z = \frac{x}{\varepsilon_2} \tag{5}$$

Moreover, we assume that each property of a material is y and z periodic functions in Y and Z, respectively. Thus, we assume that the desired solution can be represented as a power series in terms of small parameters ε_1 and ε_2, namely

$$u_\varepsilon(x, y, z) = \tilde{u}(x) + \sum_{i=1}^{\infty} u_i(x, y)\varepsilon_1^i + \sum_{i=1}^{\infty} u_i^*(y, z)\varepsilon_2^i \tag{6}$$

Since the quantities involved vary in scale y and z, the following cell averaging operators are defined

$$\langle \bullet \rangle_y = \frac{1}{|Y|} \int_Y \bullet \, dy \quad \text{and} \quad \langle \bullet \rangle_z = \frac{1}{|Z|} \int_Z \bullet \, dz,$$

where $|Y|$ and $|Z|$ represent periodic cell sizes.

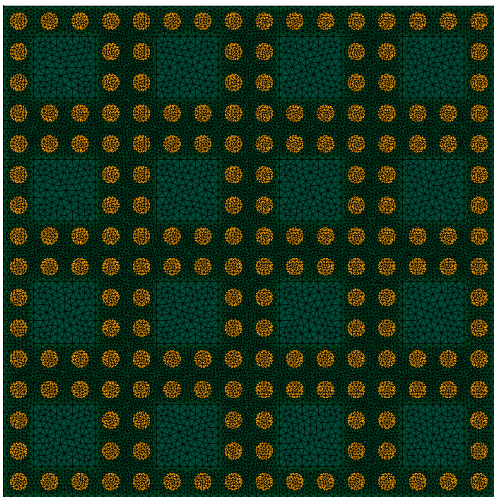

Figure 2. Overview of the finite element approximation mesh.

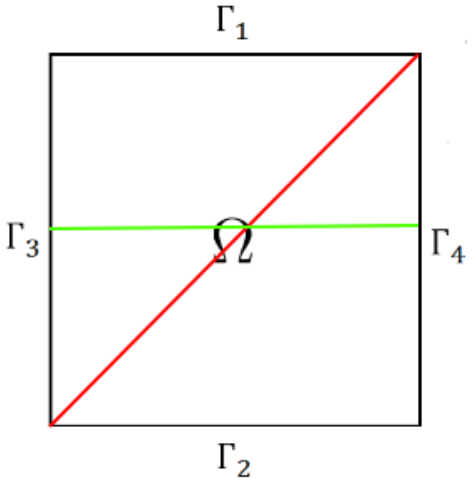

Figure 3. Computational domain.

3. Numerical experiment

Due to the fact that it is too difficult to obtain a theoretical solution to this problem (1),we will replace our exact solution with the finite element approximation obtained on a very fine mesh. Were selected linear triangular elements for the original problem on a very fine mesh for the reference solution and the same elements for the coarse mesh. For this study, as a coarse mesh was chosen unit area broken into rectangles, which in turn are divided into four elements.

To demonstrate the thermal conductivity properties in porous materials with multiple configurations, the effective thermal conductivity coefficients were calculated, which are equal for the classical two-scale asymptotic homogenization

$$\mathcal{A}^H = \begin{pmatrix} 0.265618330939 & 5.6792373e-05 \\ 5.6792373e-05 & 0.265617481342 \end{pmatrix}$$

and three-scale asymptotic homogenization

$$\mathcal{A}_Y^H = \begin{pmatrix} 0.160221931759 & 7.4758127e-05 \\ 7.4758127e-05 & 0.160221880602 \end{pmatrix},$$

$$\mathcal{A}_Z^H = \begin{pmatrix} 0.269216950836 & 0.000212804424 \\ 0.000212804424 & 0.269216950836 \end{pmatrix}$$

micro and meso scales respectively.

We also calculated L^2 and H^1 error norms for two-scale and three-scale asymptotic homogenization technique, which are presented in the tables 1 and 2.

For numerical studies were selected case where $k_1 = 0.1$ W/(m$\cdot K$), $k_2 = 1.0$ W/(m$\cdot K$), $k_3 = 10.0$ W/(m $\cdot$ K), $T(\mathbf{x}) = 0.0$, $\mathbf{x} \in \Gamma_i, i = 1, 2, 3, 4$ and with heat source $f = 8.0$ W/m^3. Calculated temperature fields are shown in Figures 5, 6 and 7. For clarity, the contour lines are also presented in the same place for all three solutions compared to each other in the Figure 4.

In the case of two-scale asymptotic homogenization, we get 2.4% of relative error, for three-scale asymptotic homogenization, the relative error equals 3.7%. This is explained by the fact that for asymptotic homogenization, the periodicity of the cells is important, i.e.

$$\lim_{\varepsilon \to 0} ||\mathcal{E}_{rel}||_{L^2} \longrightarrow 0$$

Table 1. Absolute and relative error norms for two-scale asymptotic homogenization

Coarse grid	$\|\|\mathcal{E}_{rel}\|\|_{L^2}$ (%)	$\|\|\mathcal{E}_{rel}\|\|_{H^1}$ (%)
4x4	16.012	126.913
8x8	7.744	88.818
16x16	4.764	70.670
32x32	3.280	55.001
64x64	2.584	28.264
128x128	2.513	18.747
256x256	2.491	12.193
512x512	2.488	11.051

Table 2. Absolute and relative error norms for three-scale asymptotic homogenization

Coarse grid	$\|\|\mathcal{E}_{rel}\|\|_{L^2}$ (%)	$\|\|\mathcal{E}_{rel}\|\|_{H^1}$ (%)
4x4	16.723	128.977
8x8	8.412	90.395
16x16	5.452	72.112
32x32	4.252	56.540
64x64	3.732	30.512
128x128	3.680	21.924
256x256	3.665	16.898
512x512	3.663	15.947

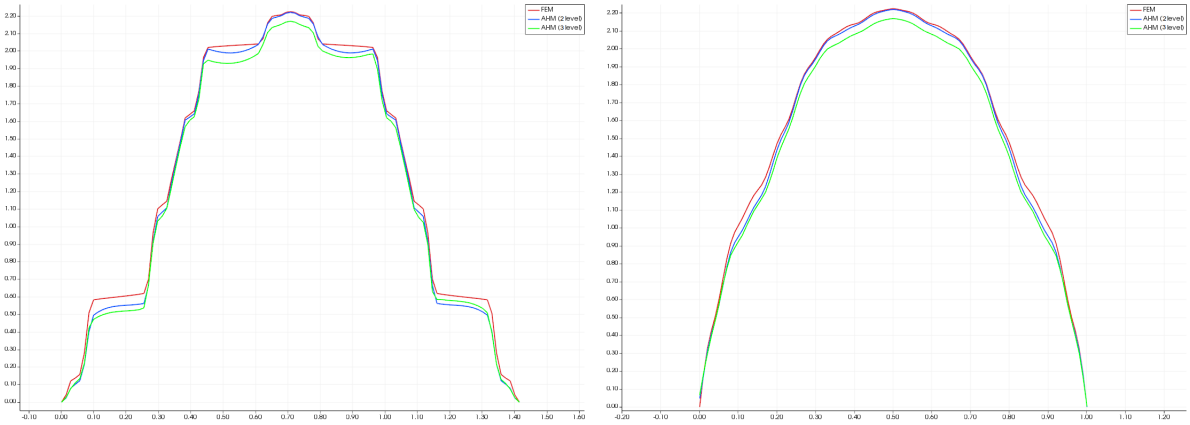

Figure 4. Diagonal and transverse isolines

Details about this can be found in the following papers [10–14]. In this paper, we have chosen a small periodicity. With large periodicities, both of these methods show good accuracy.

4. Conclusion

It is obvious that the use of the usual finite-element approximation on a grid that resolves the entire heterogeneity of the material is very expensive in terms of computing resources. In

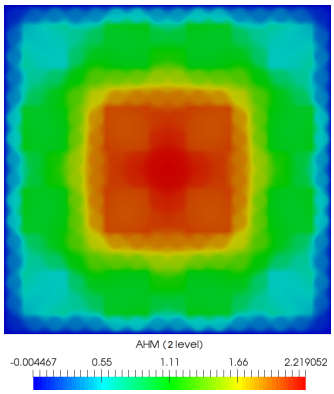

Figure 5. Two-scale asymptotic homogenization.

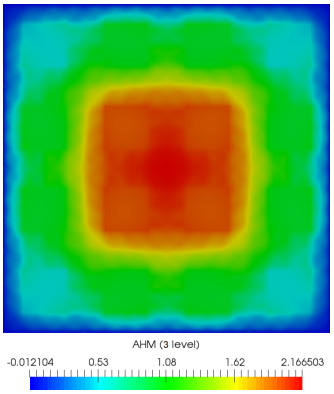

Figure 6. Three-scale asymptotic homogenization.

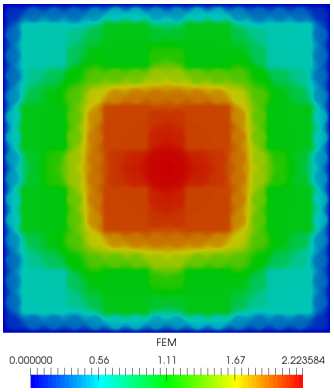

Figure 7. Finite element approximation

the case of a three-scale asymptotic homogenization, the scale separation provides undeniable advantages in reducing computational complexity. Also, this approach is a useful tool not only for calculating the thermophysical properties of composite materials, but also for studying biomechanical and engineering applications in which there are several length scales. Thus, the scale separation is the first step to computationally executable multiscale modeling of complex hierarchical materials.

Acknowledgments

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