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

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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 heterogenities. 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.
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 $\varepsilon \to 0$

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

(1)

$$u_\varepsilon(x) = 0, \quad x \in \partial \Omega,$$

(2)

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

$$a_\varepsilon(x + k(\varepsilon L)e_i) = a_\varepsilon(x), \quad \forall k \in \mathbb{Z}, \quad i = \{1, 2\},$$

(3)

where $e_i$ 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.

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

(4)

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

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

(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 $\varepsilon_1$ and $\varepsilon_2$, namely

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

(6)

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

$$(\bullet)_y = \frac{1}{|Y|} \int_Y \bullet \, dy \quad \text{and} \quad (\bullet)_z = \frac{1}{|Z|} \int_Z \bullet \, dz,$$

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

\[ A_H^\text{H} = \begin{pmatrix} 0.265618330939 & 5.6792373e - 05 \\ 5.6792373e - 05 & 0.265617481342 \end{pmatrix} \]

and three-scale asymptotic homogenization

\[ A_Y^\text{H} = \begin{pmatrix} 0.160221931759 & 7.4758127e - 05 \\ 7.4758127e - 05 & 0.160221880602 \end{pmatrix}, \]

\[ A_Z^\text{H} = \begin{pmatrix} 0.269216950836 & 0.000212804424 \\ 0.000212804424 & 0.269216950836 \end{pmatrix} \]

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 \( k_1 = 0.1 \text{ W/(m} \cdot \text{K)} \), \( k_2 = 1.0 \text{ W/(m} \cdot \text{K)} \), \( k_3 = 10.0 \text{ W/(m} \cdot \text{K)} \), \( T(\mathbf{x}) = 0.0 \), \( \mathbf{x} \in \Gamma_i, i = 1, 2, 3, 4 \) and with heat source \( f = 8.0 \text{ W/m}^3 \).

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.

\[ \lim_{\varepsilon \to 0} \| \mathbf{E}_{rel} \|_{L^2} \rightarrow 0 \]
Table 1. Absolute and relative error norms for two-scale asymptotic homogenization

| Coarse grid | $||E_{rel}\||_{L^2}$ (%) | $||E_{rel}\||_{H^1}$ (%) |
|-------------|-------------------------|-------------------------|
| 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 | $||E_{rel}\||_{L^2}$ (%) | $||E_{rel}\||_{H^1}$ (%) |
|-------------|-------------------------|-------------------------|
| 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
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.

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References
[1] Bensoussan A, Lions J L and Papanicolaou G 2011 Asymptotic analysis for periodic structures vol 374 (American Mathematical Soc.)
[2] Cioranescu D and Donato P 1999
[3] Oleinik O A, Shamaev A and Yosifian G 2009 Mathematical problems in elasticity and homogenization vol 2 (Elsevier)
[4] Jikov V V, Kozlov S M and Oleinik O A 2012 Homogenization of differential operators and integral functionals (Springer Science & Business Media)
[5] Temizer I and Wriggers P 2011 Journal of the Mechanics and Physics of Solids 59 344–372
[6] Li Z H, Ma Q and Cui J 2016 Journal of Computational Physics 314 712–748
[7] Zhang H, Zhang S, Bi J Y and Schrefler B 2007 International Journal for Numerical Methods in Engineering 69 87–113
[8] Fish J, Yu Q and Shek K 1999 International journal for numerical methods in engineering 45 1657–1679
[9] Alexandre R 1997 Proceedings of the Royal Society of Edinburgh Section A: Mathematics 127 441–455
[10] Allaire G 1992 SIAM Journal on Mathematical Analysis 23 1482–1518
[11] Allaire G 1994 PITMAN RESEARCH NOTES IN MATHEMATICS SERIES 1–1
[12] Trucu D, Chaplain M and Marciniak-Czochra A 2012 Applicable Analysis 91 1351–1373