Fraunhofer Institut Techno- und Wirtschaftsmathematik

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Berichte des Fraunhofer ITWM, Nr. 132 (2008)

ISSN 1434-9973

Bericht 132 (2008)

Die Veröffentlichungen in der Berichtsreihe des Fraunhofer ITWM können bezogen werden über:

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Vorwort

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Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

AN EFFICIENT APPROACH FOR UPSCALING PROPERTIES OF COMPOSITE MATERIALS WITH HIGH CONTRAST OF COEFFICIENTS

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ABSTRACT. An efficient approach for calculating the effective heat conductivity for a class of industrial composite materials, such as metal foams, fibrous glass materials, and the like, is discussed. These materials, used in insulation or in advanced heat exchangers, are characterized by a low volume fraction of the highly conductive material (glass or metal) having a complex, network-like structure and by a large volume fraction of the insulator (air). We assume that the composite materials have constant macroscopic thermal conductivity tensors, which in principle can be obtained by standard up-scaling techniques, that use the concept of representative elementary volumes (REV), i.e. the effective heat conductivities of composite media can be computed by post-processing the solutions of some special cell problems for REVs. We propose, theoretically justify, and numerically study an efficient approach for calculating the effective conductivity for media for which the ratio δ of low and high conductivities satisfies $\delta \ll 1$. In this case one essentially only needs to solve the heat equation in the region occupied by the highly conductive media. For a class of problems we show, that under certain conditions on the microscale geometry, the proposed approach produces an upscaled conductivity that is $\mathcal{O}(\delta)$ close to the exact upscaled permeability. A number of numerical experiments are presented in order to illustrate the accuracy and the limitations of the proposed method. Applicability of the presented approach to upscaling other similar problems, e.g. flow in fractured porous media, is also discussed.

Keywords: effective heat conductivity, permeability of fractured porous media, numerical upscaling, fibrous insulation materials, metal foams.

1. Introduction

The upscaled properties of composite materials/media, such as effective heat or electrical conductivities of composite materials, the effective permeabilities of porous media, etc. are in strong demand in engineering, geoscience, and environmental studies to name just a few. Below, we will mainly discuss calculating the effective heat conductivity, having in mind that electrical conductivity, and meso- to macro-scale upscaling in saturated porous media, lead to the same mathematical problems.

It is well known, that for heterogeneous media, for which the length-scale of the heterogeneity is small compared to some macroscopic length-scale, it is often possible to extract some effective property describing the media on the macroscopic length-scale. The mathematical framework in which this determination of effective properties is carried out is the theory of homogenization. Two instances which have been studied detailedly are the cases when the small scale heterogeneities are either periodic or statistically homogeneous. (For details on homogenization theory we would like to refer the reader to [JKO94, Tor02, WEH02], and the references therein.) In both cases the effective properties can be deduced by solving suitable sets of "cell" problems on representative elementary volumes (REV). For a periodic and for a statistically homogeneous structure, a periodicity cell and a sufficiently large (compared with the length-scale of the heterogeneity) sample, constitutes an REV, respectively. For a discussion of the definition of an REV and for a derivation and justification of the homogenization procedure, we refer the reader to [JKO94, BP04, Hor97], and to the references therein.

In this paper the equation under consideration is the stationary heat equation. Assume that we are given an REV V, which is an open domain in $\mathbb{R}^n$. According to [JKO94, WEH02, Tor02, Hor97] the effective thermal conductivity tensor $\tilde{K}$ of V can be deduced by post-processing n solutions $u_i,\ i = 1, \dots, n$ of

$$\nabla \cdot (K \nabla u_i) = 0, \text{ in } V, \tag{1}$$

where the conductivity $K = K(\boldsymbol{x})$ may vary on a small length-scale, and where the u_i satisfy suitable boundary conditions. For simplicity let us assume, that V is brick shaped, and that its faces are parallel to the coordinate planes. In the literature, four choices of boundary conditions of the "cell" problems are used in connection with numerical upscaling, namely, periodic, linear drop, linear drop and no-flow, and oscillatory boundary conditions. For a discussion of these different kinds of boundary conditions used for upscaling periodic and statistically homogeneous media see e.g. [WEH02, HWC99, BP04]. In this paper we only consider the case of linear drop boundary conditions, i.e.

$$u_i = x_i \quad \text{on } \Gamma, \tag{2}$$

where x_i is the i-th component of $\boldsymbol{x} = (x_1, \dots, x_n)$.

With $u_i,\ i = 1, \dots, n$ solving (1)-(2) we obtain the effective conductivity $\tilde{K}$ by

$$\tilde{K} \boldsymbol{e}_i = - \langle \boldsymbol{\phi}_i \rangle_V, \tag{3}$$

where $\boldsymbol{\phi}_i := -K \nabla u_i$ and $\langle \cdot \rangle_V$ denotes the volume average over V (cf. [WEH02]).

The aim of this paper is to propose and to justify an efficient approach for calculating the effective thermal conductivities $\tilde{K}$ for a specific important class of composite materials and porous media. The composite materials/media we consider are characterized by

- a high contrast of the conductivities of the constituents,
- a large volume fraction of the poorly conductive constituent,
- a low volume fraction of the highly conductive constituent,
- the highly conductive constituent forming a network with complex internal structure.

Examples for such composite materials are some industrial metal and glass foams, fibrous metal and glass materials, and the like, which are widely used in insulation or in advanced heat exchangers. These materials are characterized by a very complex internal structure, by a low volume fraction of the highly conductive material (glass or metal), and by a large volume fraction of the air. Another instance are fractured porous media, where the fractures usually occupy only a very small fraction of the domain.

There exists an extensive literature on analytical and numerical approaches for calculating effective heat conductivities for composite materials by solving (1)-(2), e.g. [JKO94, WEH02, Tor02, WZ06, ...], to mention just a few. In fact, (1)-(2) state a Dirichlet problem for an elliptic equation with (highly) varying coefficients.

Among the optimal iterative methods for solving such problems are multigrid methods (MG) (see, e.g., [Bra02, Hac03, Bra93]), algebraic multilevel iterative methods (AMLI) (see, e.g., [AV00, ...]), and domain decomposition methods (DD) (see, e.g., [TW05, ...]). In the case of highly varying coefficients, the discretization of (1)-(2) leads to a system of linear algebraic equations with a large condition number. Therefore, we relate our approach to those iterative methods for which the convergence does not depend on the contrast of the coefficients. In the case of piecewise constant conductivities, a special Domain Decomposition method has a convergence rate which does not depend on the contrast of the coefficients, see [TW05, Nep91]. In this case the subdomains are chosen so that each of them is occupied by only one of the materials.

Our approach can be viewed as a further development of this idea. Note, that unlike in the standard situation, we do not need the solution of (1)-(2), but we only need its functional defined in (3). We will show that $\tilde{K}$ can be approximated reasonably well by post-processing the solution of a problem which is only posed on the highly conductive components, which are assumed to have a network-like structure and a low volume fraction. Specifically, we would like to point out, that unlike in many other domain decomposition methods, we do not need to perform any iterations between subdomains corresponding to highly and lowly conductive regions, respectively.

The remainder of the paper at hand is organized as follows: The motivation to replace solving (1)-(2) in the entire REV by solving a derived problem in the subdomain occupied by the highly conductive material is presented in the next section. The third section concerns a theoretical justification of such an approach. In particular it is proven, that an $\mathcal{O}(\delta)$ approximation to $\tilde{K}$ can be computed in this efficient way. The resulting algorithm is described in the fourth section. The fifth section contains results from numerical experiments confirming the theoretical derivations as well as the conclusions.

2. An approach for upscaling high-contrast media

In this paper our main objective is to efficiently compute an approximation of the effective thermal conductivity tensor $\tilde{K}$ for a high contrast medium, based on the assumption, that the underlying sample V constitutes an REV. The term "high contrast" refers to the fact, that the conductivities in V vary significantly in magnitude.

As we will show, the task of computing an approximation of $\tilde{K}$ reduces to the problem of finding approximations to $u_i,\ i = 1, \dots, n$ restricted to the highly conductive parts of V.

At this point it should be emphasized, that we don't investigate the question whether for given V and K it is actually reasonable to seek the effective thermal conductivity tensor. In certain situations such an effective material property doesn't exist. Regardless of this problem the analysis carried out in Section 3 holds true. Nevertheless, the main application of our derivations is the efficient computation of effective thermal conductivity tensors for high contrast media, which of course only makes sense, if such an effective material property exists, i.e. V is an REV.

For problems with (very) high contrasts, the discretization of equation (1) together with (2) may be very hard to solve numerically due to a large condition number of the arising stiffness matrix. Besides, the mere size of the domain under consideration may lead to difficulties, since the number of unknowns in the resulting linear system can easily exceed the capacity of modern computer architectures.

Let us for simplicity assume that our conductivity K is a scalar function, which only takes two distinct values K_A and K_M, with $K_A \ll K_M$. The idea to tackle this problem is to decompose our domain V into two subsets V_A and V_M with low and with high conductivity, respectively (the subindices A and M stand for "air" and "metal", respectively).

With this decomposition, equation (3) can be written as

$$\tilde{K}\boldsymbol{e}_i = \frac{|V_A|}{|V|}\left\langle K_A \nabla u_i \right\rangle_{V_A} + \frac{|V_M|}{|V|}\left\langle K_M \nabla u_i \right\rangle_{V_M}. \tag{4}$$

(Here and in the following $|\cdot|$, when applied to sets, denotes the Lebesgue measure - the dimension being clear from context.)

Now, we may of course w.l.o.g. suppose that $K_M = 1$ and $K_A = \delta$ (simply divide (1) by K_M). By our assumptions $\delta \ll 1$. With this change in notation we obtain

$$\tilde{K}\boldsymbol{e}_i = \delta\frac{|V_A|}{|V|}\left\langle \nabla u_i \right\rangle_{V_A} + \frac{|V_M|}{|V|}\left\langle \nabla u_i \right\rangle_{V_M}. \tag{5}$$

Now, it would of course be very desirable to compute $u_i|_{V_M}$ by solving a constant coefficient problem and then to compute (an approximation to) $\tilde{K}$ from $u_i|_{V_M}$. The justification for such an approach can be motivated as follows:

By assumption we know that the conductivity in V_M is much larger than the one in V_A, i.e. $\delta \ll 1$. Therefore, the coupling within a path-connected component of V_M is much larger than the coupling of this component with the adjacent parts of V_A. In other words, every path-connected component of V_M is very well insulated by the adjacent parts of V_A.

Therefore, it seems justified to approximate $u_i|_{V_M}$ by solving (1) in V_M by using homogeneous Neumann boundary conditions on the interface $\Sigma := \partial V_M \cap \partial V_A$. Thereby, we approximate the very high insulation mentioned above by perfect insulation. It should be noted that solving for $u_i|_{V_M}$ thus becomes a constant coefficient problem, which is of course much better conditioned than the problem we started with.

For very small δ it is intuitively clear that the lowly conductive part of the medium in V_A doesn't contribute significantly to the overall heat transfer through the entire sample V. Therefore, we don't even need to compute $u_i|_{V_A}$, for the first summand on the right hand side of (5) is negligibly small.

It should be noted that this idea was proposed earlier in [BER84, pg. 105-106] in connection with models for flow in fractured porous media. To the best of our knowledge, it has not be rigorously proven earlier, that this approach works. The next section is devoted to such a justification. Furthermore, the approximation suggested in [BER84, eq. III.90] to the permeability tensor still contains an undertermined geometrical factor. Combining the idea from [BER84] with homogenization theory, we obtain an efficient approach for calculating permeabilities of fractured porous media, as well as for calculating effective thermal conductivities for a class of composite materials with high contrasts of coefficients.

3. Analysis of the upscaling approach for high contrast materials

This section contains the theoretical justification of the approach outlined above. Lemma 3.1 states an auxiliary result essentially saying, that the solution of (1)-(2) is bounded in H^1-semi-norm, independently of the contrast δ. Proposition 3.2 allows us to neglect highly conductive components which are not connected to the boundary of the domain, and Proposition 3.3 provides a way to approximate the average of the heat flux inside the remaining highly conductive components, i.e. those which are connected to the boundary.

Having proved these preliminaries, we are able to show our main result, i.e. Theorem 3.4, stating, that an $\mathcal{O}(\delta)$ approximation of $\tilde{K}$ can be obtained by post-processing the solutions of constant coefficient elliptic equations in the subdomain of the highly conductive material, subject to the linear drop Dirichlet boundary conditions on the outer boundary and zero Neumann boundary conditions on the interface between air and metal.

The theory developed below concerns cell problems with boundary conditions given by (2). With some modifications it may also be used for cell problems with periodic boundary conditions, if the underlying REV is itself periodic.

Now, let us proceed by proving the first

Lemma 3.1. *Let Ω be a Lipschitz domain (e.g. $\Omega = V$), such that $\Omega = \left(\overline{\Omega_M} \cup \overline{\Omega_A}\right) \backslash \partial\Omega$, where Ω_M and Ω_A are open sets with Lipschitz boundary. Furthermore, let*

$$K(\boldsymbol{x}) = \begin{cases} K_M = 1, & \boldsymbol{x} \in \Omega_M \\ K_A = \delta, & \boldsymbol{x} \in \Omega_A. \end{cases}$$

Now, let u be the solution of

$$\begin{cases} \nabla \cdot (K(\boldsymbol{x}) \nabla u(\boldsymbol{x})) &= 0, & \boldsymbol{x} \in \Omega \\ u(\boldsymbol{x}) &= g(\boldsymbol{x}), & \boldsymbol{x} \in \partial\Omega, \end{cases} \tag{6}$$

where $g \in H^{\frac{1}{2}}(\partial\Omega)$. As an additional regularity assumption concerning Ω_M and Ω_A we require, that for each open set Ω_c which is compactly contained in Ω (i.e. $\Omega_c \subset\subset \Omega$) we have for v_M and v_A defined in (8) and (9) below, respectively, that $v_M|_{\Omega_c \cap \Omega_M} \in H^2(\Omega_c \cap \Omega_M)$ and $v_A|_{\Omega_c \cap \Omega_A} \in H^2(\Omega_c \cap \Omega_A)$.

Then, for all δ we have that

$$\|\nabla u\|_{L^2(\Omega)} \leq C. \tag{7}$$

(Here and in the following C denotes a generic constant independent of δ.)

Proof. First, we construct an auxiliary function $v \in H^1(\Omega)$ as follows: $v_M := v|_{\Omega_M}$ solves

$$\begin{cases} \nabla \cdot (K_M \nabla v_M(\boldsymbol{x})) &= 0, & \boldsymbol{x} \in \Omega_M \\ v_M(\boldsymbol{x}) &= g(\boldsymbol{x}), & \boldsymbol{x} \in \partial\Omega \cap \partial\Omega_M \\ \frac{\partial v_M(\boldsymbol{x})}{\partial \boldsymbol{n}} &= 0, & \boldsymbol{x} \in \Sigma \end{cases} \tag{8}$$

(Here $\boldsymbol{n}(\boldsymbol{x})$, $\boldsymbol{x} \in \Sigma$ denotes the outer unit normal vector.) and $v_A := v|_{\Omega_A}$ solves

$$\begin{cases} \nabla \cdot (K_A \nabla v_A(\boldsymbol{x})) &= 0, & \boldsymbol{x} \in \Omega_A \\ v_A(\boldsymbol{x}) &= g(\boldsymbol{x}), & \boldsymbol{x} \in \partial\Omega \cap \partial\Omega_A \\ v_A|_\Sigma &= v_M|_\Sigma. \end{cases} \tag{9}$$

(Note, that the solutions to (8) and (9) are actually independent of K.) Now, choose $w \in C_0^\infty(\Omega)$ and let Ω_c be such that $supp(w) \subset \Omega_c$. Then, due to our regularity assumptions on v_M and v_A we have

(10)
$$\begin{aligned}
\int_\Omega K\nabla v \cdot \nabla w d\boldsymbol{x} &= \int_{\Omega_c} K\nabla v \cdot \nabla w d\boldsymbol{x} \\
&= \sum_{E\in\{A,M\}} \int_{\Omega_E\cap\Omega_c} K_E \nabla v_E \cdot \nabla w d\boldsymbol{x} \\
&= \sum_{E\in\{A,M\}} \left(-\int_{\Omega_E\cap\Omega_c} \underbrace{\nabla\cdot(K_E\nabla v_E)}_{=0} w d\boldsymbol{x} + \int_{\partial(\Omega_E\cap\Omega_c)} K_E \frac{\partial v_E}{\partial \boldsymbol{n}} w dS(\boldsymbol{x}) \right) \\
&= \int_{\Sigma\cap\Omega_c} \delta \frac{\partial v_A}{\partial \boldsymbol{n}_\Sigma} w dS(\boldsymbol{x}) \\
&= \int_\Sigma \delta \frac{\partial v_A}{\partial \boldsymbol{n}_\Sigma} w dS(\boldsymbol{x}),
\end{aligned}$$

where we have used Green's formula, $\left.\frac{\partial v_M(\boldsymbol{x})}{\partial \boldsymbol{n}}\right|_\Sigma = 0$, and $supp(w) \subset \Omega_c$. Here, $\boldsymbol{n}_\Sigma$ denotes the unit normal vector pointing from Ω_A to Ω_M. By a standard density argument we obtain the validity of (10) for all $w \in H_0^1(\Omega)$.

Since u solves (6) we have for all $w \in H_0^1(\Omega)$

$$\int_\Omega K\nabla u \cdot \nabla w d\boldsymbol{x} = 0. \tag{11}$$

Subtracting (11) from (10) yields

$$\begin{aligned}
\int_\Omega K\nabla(v-u)\cdot\nabla w d\boldsymbol{x} &= \int_\Sigma \delta \frac{\partial v_A}{\partial \boldsymbol{n}_\Sigma} w dS(\boldsymbol{x}) \\
&\le \delta \left\| \frac{\partial v_A}{\partial \boldsymbol{n}_\Sigma} \right\|_{H^{-\frac{1}{2}}(\Sigma)} \|w\|_{H^{\frac{1}{2}}(\Sigma)} \\
&\le C\delta \|w\|_{H^{\frac{1}{2}}(\Sigma)},
\end{aligned} \tag{12}$$

where we have used the Cauchy-Schwarz inequality and the fact, that $\left\| \frac{\partial v_A}{\partial \boldsymbol{n}_\Sigma} \right\|_{H^{-\frac{1}{2}}(\Sigma)}$ is independent of δ. Choosing $w = v - u \in H_0^1(\Omega)$ and noting that $K \ge \delta$ we obtain

$$\int_\Omega \delta\nabla(v-u)\cdot\nabla(v-u)\, d\boldsymbol{x} \le C\delta \|v-u\|_{H^{\frac{1}{2}}(\Sigma)}.$$

Using the trace theorem and the Poincaré inequality we deduce

$$\int_\Omega \nabla(v-u)\cdot\nabla(v-u)\, d\boldsymbol{x} \le C\|\nabla(v-u)\|_{L^2(\Omega)}. \tag{13}$$

Thus,

$$\|\nabla(v-u)\|_{L^2(\Omega)} \le C, \tag{14}$$

which implies (7), because v is independent of δ. □

The previous lemma plays a key role in the development of the further theory. Its application in the following proposition allows us to simplify our geometry, if path-connected components of the highly conductive domain are strictly inside Ω.

Proposition 3.2. *Assume the same setting as in the statement of Lemma 3.1. Additionally, let $\widetilde{\Omega_M}$ be the union of path-connected components of Ω_M that don't touch the boundary, i.e. $|\partial\widetilde{\Omega_M} \cap \partial\Omega| = 0$. Then*

$$\left| \langle \boldsymbol{\phi} \rangle_\Omega - \frac{|\Omega^*|}{|\Omega|} \langle \boldsymbol{\phi} \rangle_{\Omega^*} \right| = \mathcal{O}(\delta), \text{ as } \delta \to 0, \tag{15}$$

where as above $\boldsymbol{\phi} = -K\nabla u$ and $\Omega^* :=$ interior $\left(\Omega \backslash \widetilde{\Omega_M}\right)$. Here and below $|\cdot|$ applied to elements from $\mathbb{R}^n$ denotes some norm. (We refer to Figure 1 for a better understanding of the components of Ω).

Proof. It is easy to see that

$$\left| \langle \boldsymbol{\phi} \rangle_\Omega - \frac{|\Omega^*|}{|\Omega|} \langle \boldsymbol{\phi} \rangle_{\Omega^*} \right| = \frac{1}{|\Omega|} \left| \int_{\widetilde{\Omega_M}} \boldsymbol{\phi} d\boldsymbol{x} \right|. \tag{16}$$

Define $v := u|_{\widetilde{\Omega_M}}$, where u solves (6). Clearly, v is up to additive constants (one for each path-connected component of $\widetilde{\Omega_M}$) uniquely defined by

$$\begin{cases} \nabla \cdot \nabla v &= 0, \quad \text{in } \widetilde{\Omega_M} \\ \dfrac{\partial v}{\partial \boldsymbol{n}} &= \delta \dfrac{\partial u_A}{\partial \boldsymbol{n}} \quad \text{on } \partial\widetilde{\Omega_M}, \end{cases} \tag{17}$$

where $u_A = u|_{\Omega_A}$ and $\boldsymbol{n}$ is the outward normal vector of $\widetilde{\Omega_M}$. Obviously, we have that

$$\left| \int_{\widetilde{\Omega_M}} \boldsymbol{\phi} d\boldsymbol{x} \right| \le \|\boldsymbol{\phi}\|_{L^1\left(\widetilde{\Omega_M}\right)} \le C\|\boldsymbol{\phi}\|_{L^2\left(\widetilde{\Omega_M}\right)} = C\|\nabla v\|_{L^2\left(\widetilde{\Omega_M}\right)}.$$

By [GR86, Section 1.4] we know, that

$$\|\nabla v\|_{L^2\left(\widetilde{\Omega_M}\right)} \le C\delta \left\| \frac{\partial u_A}{\partial \boldsymbol{n}} \right\|_{H^{-\frac{1}{2}}\left(\partial\widetilde{\Omega_M}\right)},$$

from where we deduce by [GR86, Theorem 1.6] that

$$\|\nabla v\|_{L^2\left(\widetilde{\Omega_M}\right)} \le C\delta \|u\|_{H^1(\Omega)}.$$

Thus, we have that

$$\|\nabla v\|_{L^2\left(\widetilde{\Omega_M}\right)} \le C\delta \left(\|u\|_{L^2(\Omega)} + \|\nabla u\|_{L^2(\Omega)} \right), \tag{18}$$

and it suffices to show, that $\|u\|_{L^2(\Omega)}$ and $\|\nabla u\|_{L^2(\Omega)}$ are bounded independently of δ.

Lemma 3.1 yields that $\|\nabla u\|_{L^2(\Omega)}$ is bounded independently of δ. To make an estimate for $\|u\|_{L^2(\Omega)}$ we use the following construction: Let w be the harmonic extension of g from (6), i.e. w solves

$$\begin{cases} \nabla \cdot \nabla w &= 0, \quad \text{in } \Omega \\ w &= g, \quad \text{on } \partial\Omega. \end{cases} \tag{19}$$

By [GR86, Section 1.3] we have that

$$\|w\|_{H^1(\Omega)} \le \|g\|_{H^{\frac{1}{2}}(\partial\Omega)} < C, \tag{20}$$

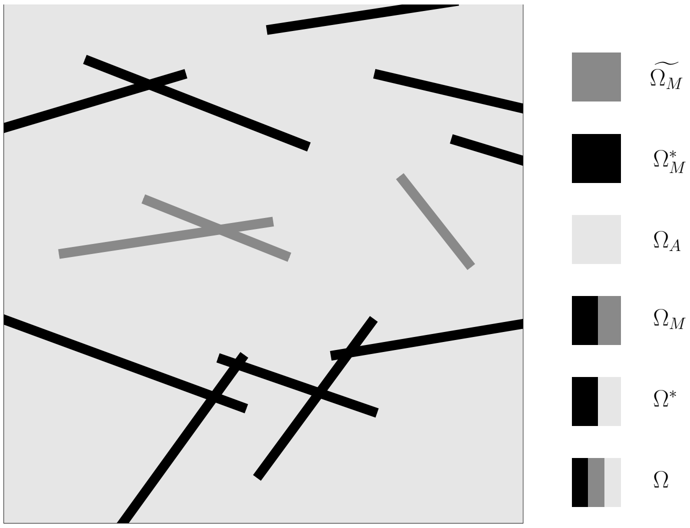


FIGURE 1. Components of Ω.

where, as usual, C is a constant independent of δ.

By Poincaré's inequality we have for $u - w \in H_0^1(\Omega)$

$$\|u - w\|_{L^2(\Omega)} \le \|\nabla u\|_{L^2(\Omega)} + \|\nabla w\|_{L^2(\Omega)} \le C, \tag{21}$$

where we have used Lemma 3.1 and the fact that w is independent of δ. (20) combined with (21) yields the uniform (w.r.t. δ) boundedness of $\|u\|_{L^2(\Omega)}$, which concludes the proof. □

Remark 3.1. Observe, that by the proof of Proposition 3.2 we have in particular that the solution u of (6) is bounded independently of δ in H^1-norm.

The meaning of Proposition 3.2 is that in the computation of the effective conductivity $\tilde{K}$ via (3) we can neglect those highly conductive path-connected components of V which don't touch the boundary of V.

The next proposition provides a means to approximate $\langle \boldsymbol{\phi} \rangle_{\Omega^*}$ by a function constructed similarly to the auxiliary function in Lemma 3.1.

Proposition 3.3. *Let the assumptions of Lemma 3.1 be satisfied. Additionally, let* $\boldsymbol{\phi}$ *and* Ω^* *be defined as in Proposition 3.2. Furthermore, let*

$$v = \begin{cases} v_M, & \text{in } \Omega_M \\ v_A, & \text{in } \Omega_A \end{cases}$$

be the solution of

$$\begin{cases} \nabla \cdot \nabla v_M = 0 & \text{in } \Omega_M \\ v_M = g & \text{on } \partial\Omega \cap \partial\Omega_M \\ \dfrac{\partial v_M}{\partial \boldsymbol{n}} = 0 & \text{on } \Sigma^* \\ v_M = u & \text{on } \Sigma \backslash \Sigma^* \end{cases} \tag{22}$$

and

$$\left\{\begin{array}{rcll}\nabla\cdot\nabla v_A & = & 0 & \text{in } \Omega_A\\ v_A & = & g & \text{on } \partial\Omega\cap\partial\Omega_A\\ v_A & = & v_M & \text{on } \Sigma^*\\ v_A & = & u\ (=v_M) & \text{on } \Sigma\backslash\Sigma^*,\end{array}\right. \tag{23}$$

where $\Sigma^* := \partial\Omega_M^*\cap\Sigma$ *and* $\Omega_M^* = \text{interior}\,(\Omega^*\backslash\Omega_A)$*. Also, we require that each path-connected component of* Ω_M^* *is a finite union of domains each of which is star-shaped w.r.t. a ball. (Note, that we already know, that by construction each path-connected component of* Ω_M^* *touches* $\partial\Omega$*.)*

Then,

$$|\langle\boldsymbol{\phi}\rangle_{\Omega^*} - \langle\boldsymbol{\psi}\rangle_{\Omega^*}| = \mathcal{O}(\delta)\,,\quad \text{as } \delta\to 0, \tag{24}$$

where $\boldsymbol{\psi} = -K\nabla v$*.*

Proof. Let $w\in H_0^1(\Omega^*)$. Then similarly to (10) in Lemma 3.1 we obtain

$$\int_{\Omega^*} K\nabla v\cdot\nabla w d\boldsymbol{x} = \int_{\Sigma^*}\delta\frac{\partial v_A}{\partial\boldsymbol{n}_\Sigma} w dS(\boldsymbol{x})\,. \tag{25}$$

Clearly, we have

$$\int_{\Omega^*} K\nabla u\cdot\nabla w d\boldsymbol{x} = 0, \tag{26}$$

and subtracting (26) from (25) yields

$$\int_{\Omega^*} K\nabla(v-u)\cdot\nabla w d\boldsymbol{x} = \delta\int_{\Sigma^*}\frac{\partial v_A}{\partial\boldsymbol{n}_\Sigma} w dS(\boldsymbol{x}) \le \delta\left\|\frac{\partial v_A}{\partial\boldsymbol{n}_\Sigma}\right\|_{H^{-\frac12}(\Sigma^*)}\|w\|_{H^{\frac12}(\Sigma^*)}\,. \tag{27}$$

By Remark 3.1 we know that $\|u\|_{H^1(\Omega)}\le C$, where C as throughout this paper does not depend on δ. Therefore,

$$\|v_A\|_{H^{\frac12}(\Sigma\backslash\Sigma^*)} = \|u\|_{H^{\frac12}(\Sigma\backslash\Sigma^*)} \le C \tag{28}$$

by the trace theorem. Thus,

$$\begin{array}{rcl}\|v_A\|_{H^1(\Omega_A)} & \le & C\,\|v_A\|_{H^{\frac12}(\partial\Omega_A)}\\ & \le & C\left(\|v_A\|_{H^{\frac12}(\Sigma\backslash\Sigma^*)} + \|v_A\|_{H^{\frac12}(\Sigma^*)} + \|v_A\|_{H^{\frac12}(\partial\Omega_A\cap\partial\Omega)}\right)\\ & = & C\left(\|v_A\|_{H^{\frac12}(\Sigma\backslash\Sigma^*)} + \|v_M\|_{H^{\frac12}(\Sigma^*)} + \|g\|_{H^{\frac12}(\partial\Omega_A\cap\partial\Omega)}\right)\\ & \le & C,\end{array} \tag{29}$$

where we have used [GR86, Section 1.3], (28), and the fact that $v_M|_{\Omega_M^*}$ does not depend on δ by (22).

Therefore, by [GR86, Theorem 1.6] we obtain

$$\left\|\frac{\partial v_A}{\partial\boldsymbol{n}_\Sigma}\right\|_{H^{-\frac12}(\Sigma^*)} \le C.$$

Combining this with (27) we are left with

$$\int_{\Omega^*} K\nabla(v-u)\cdot\nabla w d\boldsymbol{x} \le \delta C\,\|w\|_{H^{\frac12}(\Sigma^*)}\,. \tag{30}$$

Choosing $w = v - u \in H_0^1(\Omega^*)$ we obtain

$$\int_{\Omega^*} K\nabla (v-u) \cdot \nabla (v-u)\, d\boldsymbol{x} \leq \delta C \|v-u\|_{H^{\frac{1}{2}}(\Sigma^*)} \leq \delta C \|v-u\|_{H^1(\Omega^*_M)} \tag{31}$$

by the trace theorem. Now, due to the properties of Ω^*_M we may apply Poincaré's inequality (cf. [BS02, Section 5.3]) and obtain

$$\int_{\Omega^*_M} \nabla (v-u) \cdot \nabla (v-u)\, d\boldsymbol{x} \leq \delta C \|\nabla (v-u)\|_{L^2(\Omega^*_M)}. \tag{32}$$

Thus, another application of Poincaré's inequality yields

$$\|v-u\|_{H^1(\Omega^*_M)} \leq \|\nabla (v-u)\|_{L^2(\Omega^*_M)} = \mathcal{O}(\delta). \tag{33}$$

By the trace theorem we deduce that

$$\|v-u\|_{H^{\frac{1}{2}}(\Sigma^*)} = \mathcal{O}(\delta) \tag{34}$$

Since $v-u$ solves

$$\begin{cases} \nabla \cdot \nabla (v-u) &= 0 \quad \text{in } \Omega_A \\ v-u &= 0 \quad \text{on } (\partial\Omega \cap \partial\Omega_A) \cup (\Sigma \backslash \Sigma^*) \end{cases}$$

and $(\partial\Omega \cap \partial\Omega_A) \cup (\Sigma\backslash\Sigma^*) \cup \Sigma^* = \partial\Omega_A$ we have by [GR86, Section 1.3] and (34)

$$\|v-u\|_{H^1(\Omega_A)} \leq C\|v-u\|_{H^{\frac{1}{2}}(\Sigma^*)} = \mathcal{O}(\delta). \tag{35}$$

From (33) and (35) it is straight-forward to obtain (24) □

We are now ready to state our main result:

Theorem 3.4. *Let the assumptions of Lemma 3.1 be satisfied. Furthermore, let Ω^*, Σ^*, and Ω^*_M be defined as in Propositions 3.2 and 3.3, respectively. As in the previous proposition we also have to assume that each path-connected component of Ω^*_M is a finite union of domains each of which is star-shaped w.r.t. a ball. Then, if v_M solves*

$$\begin{cases} \nabla \cdot \nabla v_M &= 0 \quad \text{in } \Omega^*_M \\ v_M &= g \quad \text{on } \partial\Omega^*_M \cap \partial\Omega \\ \dfrac{\partial v_M}{\partial \boldsymbol{n}} &= 0 \quad \text{on } \Sigma^* \end{cases} \tag{36}$$

we have that

$$\left| \langle \boldsymbol{\phi} \rangle_\Omega - \frac{|\Omega^*_M|}{|\Omega|} \langle \boldsymbol{\psi} \rangle_{\Omega^*_M} \right| = \mathcal{O}(\delta), \quad \text{as } \delta \to 0, \tag{37}$$

where $\boldsymbol{\phi} = -K\nabla u$ and $\boldsymbol{\psi} = -K\nabla v$.

Remark 3.2. Before we proceed with the proof of Theorem 3.4 we note, that (37) combined with (3) provides a way to efficiently compute an approximation of the effective thermal conductivity tensor for high contrast media.

Proof. Let v be as in Proposition 3.3 (note, that then v satisfies in particular (36)). By the triangular inequality we have

$$\left|\langle\boldsymbol{\phi}\rangle_\Omega - \frac{|\Omega_M^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega_M^*}\right| \leq$$
$$\leq \underbrace{\left|\langle\boldsymbol{\phi}\rangle_\Omega - \frac{|\Omega^*|}{|\Omega|}\langle\boldsymbol{\phi}\rangle_{\Omega^*}\right|}_{=\mathcal{O}(\delta),\ \text{Prop. 3.2}} + \underbrace{\left|\frac{|\Omega^*|}{|\Omega|}\langle\boldsymbol{\phi}\rangle_{\Omega^*} - \frac{|\Omega^*|}{\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega^*}\right|}_{=\mathcal{O}(\delta),\ \text{Prop. 3.3}} + \left|\frac{|\Omega^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega^*} - \frac{|\Omega_M^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega_M^*}\right|.$$

Therefore, it suffices to show

$$\left|\frac{|\Omega^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega^*} - \frac{|\Omega_M^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega_M^*}\right| = \mathcal{O}(\delta)\,. \tag{38}$$

Observe, that

$$\begin{aligned} \frac{|\Omega^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega^*} &= \frac{1}{|\Omega|}\left(\int_{\Omega_M^*} -\nabla v d\boldsymbol{x} - \int_{\Omega_A}\delta\nabla v d\boldsymbol{x}\right) \\ &= \frac{1}{|\Omega|}\int_{\Omega_M^*} -\nabla v d\boldsymbol{x} + \mathcal{O}(\delta)\,, \quad \text{by (29)} \\ &= \frac{|\Omega_M^*|}{|\Omega|}\langle\boldsymbol{\psi}\rangle_{\Omega_M^*} + \mathcal{O}(\delta)\,, \end{aligned} \tag{39}$$

which yields (38). □

4. An efficient algorithm for high-contrast materials

Theorem and remark 3.2, provide the theoretical justification of an algorithm, which can be used to efficiently compute an approximation of the effective thermal conductivity tensor of an REV V consisting of a highly conductive (V_M) and a lowly conductive (V_A) part, where the conductivity K_M in V_M is much larger than the conductivity K_A in V_A. As stated above, we are typically interested in those materials for which $|V_M|$ is significantly smaller than $|V_A|$. The less this assumption is satisfied the less efficient the following algorithm will work. Nevertheless, even if $|V_M|$ is of the same size as $|V_A|$ - or even larger - the theory presented above applies and the algorithm below will work - just not particularly efficiently.

Note, that due to equation (39) we see that the flux in Ω_A is $\mathcal{O}(\delta)$ and may, therefore, be asymptotically neglected as $\delta \to 0$. By the proof of Proposition 3.2 we know that the same is true for the flux in $\widetilde{\Omega_M}$. Nevertheless, instead of disregarding Ω_A and $\widetilde{\Omega_M}$ completely in the calculation of the effective thermal conductivity tensor, we may of course prescribe some constant temperature gradient in Ω_A and a temperature gradient being $\mathcal{O}(\delta)$ in $\widetilde{\Omega_M}$. Certainly, for $\delta \to 0$ the resulting fluxes tend to zero, as well. Nonetheless, for a specific choice for δ we may still hope to (and in many numerically tested cases do) obtain better estimates of the effective thermal conductivity tensors. In the numerical examples presented in section 5 the temperature in Ω_A is approximated by linearly interpolating the (Dirichlet) boundary conditions, leading to a constant approximation of the temperature gradient. The temperature gradient in $\widetilde{\Omega_M}$ is obtained in the same way and then scaled by δ.

Based on our considerations above, we may now formulate Algorithm 1 for computing an approximation $\tilde{K}^{CO}$ of $\tilde{K}$ for high contrast REV's (here ^{CO} stands for "conductive only").

Algorithm 1 Compute an approximation $\tilde{K}^{CO}$ of $\tilde{K}$ for high contrast REV's

Let V be as described in Section 1 (i.e. brick shaped and with its faces parallel to the coordinate planes), and let V_M and V_A be such that $V = V_M \cup V_A$ (Note, that unlike above we do not distinguish between open and closed sets, since numerically they are treated identically.).
Let K_M and K_A be the conductivities in V_M and V_A, respectively, where $K_M \gg K_A$.
Construct a voxelized grid that resolves V_M and V_A.
Determine all connected components $V_{M,j}$, $j \in J_M$ of V_M that have a non-empty intersection with ∂V, i.e. $V_{M,j} \cap \partial V \neq \emptyset$. (Here, ∂V denotes the outermost layer of voxels in V, and J_M denotes a suitable index set.) (For a better understanding of the introduced components we refer to Figure 2.)
Set $\widetilde{V_M} = V_M \setminus \left(\bigcup_{j \in J_M} V_{M,j} \right)$.
for i=1,...,n **do**
  for $j \in J_M$ **do**
    Solve a finite volume discretization of

$$\left\{ \begin{array}{rcll} \nabla \cdot \nabla v_i & = & 0 & \text{in } V_{M,j} \\ \dfrac{\partial v_i}{\partial \boldsymbol{n}} & = & 0 & \text{on } \partial V_{M,j} \setminus \partial V \\ v_i & = & x_i & \text{on } \partial V_{M,j} \cap \partial V \quad (\neq \emptyset \text{ by construction}) \, . \end{array} \right. \tag{40}$$

  end for
  Set

$$\tilde{K}^{CO} \boldsymbol{e}_i = \frac{-1}{|V|} \left(K_M \sum_{j \in J_M} \int_{V_{M,j}} \nabla v_i d\boldsymbol{x} + K_A \left(|V_A| + |\widetilde{V_M}| \right) \boldsymbol{e}_i \right) . \tag{41}$$

end for
return $\tilde{K}^{CO}$

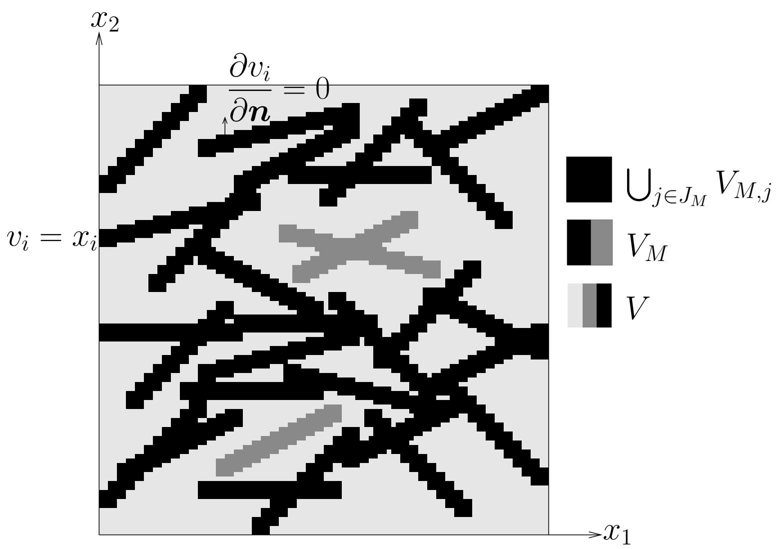


FIGURE 2. Voxelized approximation of Ω and its components.

5. Numerical Experiments and Conclusions

We now test Algorithm 1 on two fiber geometries with a sequence of increasing contrasts, i.e. decreasing δ. The fiber structures shown in Figures 3(a) and 4(a) were generated and plotted with the GeoDict2007 software[1].

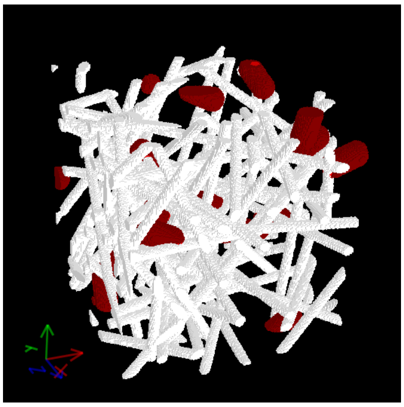
Both fiber structures are cubic and have the same solid volume fraction of 10%. 80% of the fiber volume is occupied by long thin fibers (colored white), whereas the remaining 20% are taken up by short thick fibers (colored red). The only difference in the parameters set in GeoDict2007 to generate the fiber geometries is that the structure in Figure 3(a) is isotropic, whereas the one in Figure 4(a) is anisotropic. Both geometries are discretized by 200^3 voxels.

In this context we would like to point out, that we do not make any statement concerning the question whether the structures shown in Figures 3(a) and 4(a) constitute REVs. In particular we do not claim, that (physically meaningful) effective thermal conductivity tensors exist for both structures and all considered contrasts. Certainly, the main application of Algorithm 1 is to compute effective thermal conductivity tensors. When they exist, their approximation via Algorithm 1 is very much preferable over computations on the whole domain due to significant savings in memory and a much lower condition number of the resulting linear system. Nevertheless, the statement, that (37) holds is independent of the question, whether the configuration under consideration, i.e. geometry and contrast, admits the notion of an effective thermal conductivity tensor.

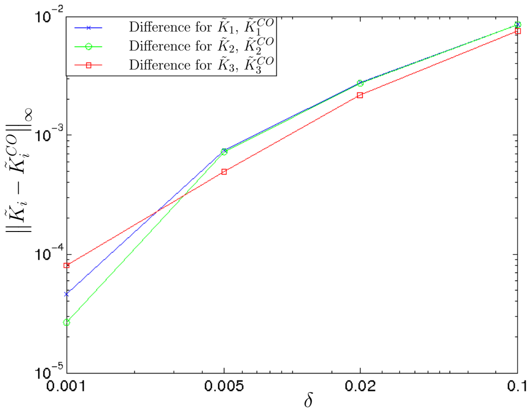
For each geometry and each δ we consider three cell problems with boundary conditions given by (2). Each boundary value problem is then solved by a standard finite volume discretization on the full domain (yielding $\tilde{K}_i := \tilde{K}\boldsymbol{e}_i$, $i = 1, 2, 3$). We then compare these reference results to the outputs given by Algorithm 1 (yielding $\tilde{K}_i^{CO} := \tilde{K}^{CO}\boldsymbol{e}_i$, $i = 1, 2, 3$). For this comparison the norm in $\mathbb{R}^3$ is chosen to be the max-norm, i.e. $|\cdot| = \|\cdot\|_\infty$ (due to equivalence of norms this choice is completely arbitrary). Figures 3(b) and 4(b) show the results for the different fiber structures, respectively.

Figures 3(b) and 4(b) suggest, that $\left\|\tilde{K}_i - \tilde{K}_i^{CO}\right\|_\infty$, $i = 1, 2, 3$, does in fact depend linearly on δ, as stated in Theorem 3.4. This verifies (37) and also suggests the optimality of this estimate. It should furthermore be noted, that the constant implicitly involved in estimate (37) appears to be rather small. From a practical point of view, this is certainly crucial. Of course, the constant is very much geometry dependent, but we can see, that for the two randomly generated fiber structures we obtain very satisfactory results even if the contrast is only $1 : 10$.

[1] For more information about this software we would like to refer the reader to the following webpage: www.geodict.com

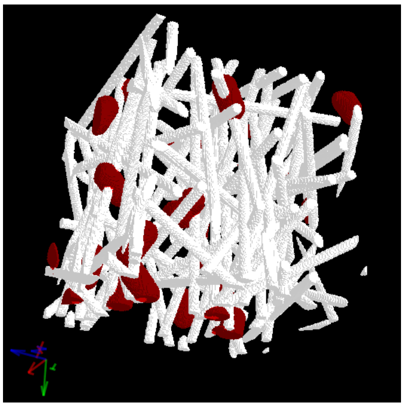


(a) Isotropic fiber structure.

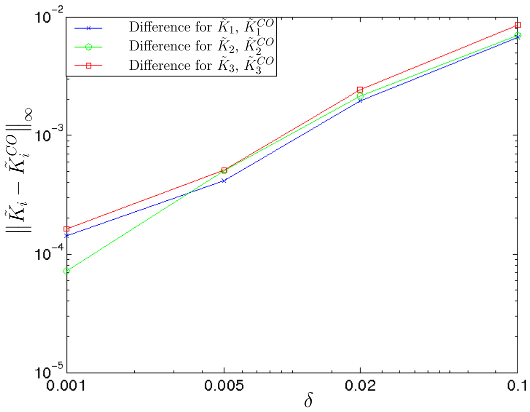


(b) Results for different contrasts.

FIGURE 3. Performance of Algorithm 1 for an isotropic fiber geometry.



(a) Anisotropic fiber structure.



(b) Results for different contrasts.

FIGURE 4. Performance of Algorithm 1 for an anisotropic fiber geometry.

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