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Vorwort

Das Tätigkeitsfeld des Fraunhofer-Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe sollen sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen werden.

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

A GRAPH-LAPLACIAN APPROACH FOR CALCULATING THE EFFECTIVE THERMAL CONDUCTIVITY OF COMPLICATED FIBER GEOMETRIES

O. ILIEV[1], R. LAZAROV[2], AND J. WILLEMS[3]

Abstract. An efficient approach to the numerical upscaling of thermal conductivities of fibrous media, e.g. insulation materials, is considered. First, standard cell problems for a second order elliptic equation are formulated for a proper piece of random fibrous structure, following homogenization theory. Next, a graph formed by the fibers is considered, and a second order elliptic equation with suitable boundary conditions is solved on this graph only. Replacing the boundary value problem for the full cell with an auxiliary problem with special boundary conditions on a connected subdomain of highly conductive material is justified in a previous work of the authors. A discretization on the graph is presented here, and error estimates are provided. The efficient implementation of the algorithm is discussed. A number of numerical experiments is presented in order to illustrate the performance of the proposed method.

Keywords: graph laplacian, effective heat conductivity, numerical upscaling, fibrous materials.

1. Introduction

A wide class of insulation materials, such as glass and mineral wool, are composed of a big number of fibers. The porosity of such materials is usually high. However, the heat conductivity of the fibers is much higher than the conductivity of the surrounding air. In a previous article, [EIL$^+$07], it was shown that the effective heat conductivity of composites containing highly conductive networks, can be calculated by solving auxiliary problems on the highly conductive subdomain only, subject to special boundary conditions. Based on this result, the thermal conductivity of the considered fibrous material is calculated over the fibers only. A graph formed by the fibers is considered, with the intersection points of the fibers being the nodes of the graph. Thus the problem for upscaling the conductivity of fibrous materials reduces to solving Laplace's equation on a graph.

According to homogenization theory, e.g. [JKO94, Tor02, WEH02, BP04], and the references therein, the effective properties of heterogeneous materials can be calculated by solving suitable sets of "cell problems" on representative elementary volumes (REV). In this paper the equation under consideration is the stationary heat equation. Assume that we are given an REV Ω, which is an open domain in $\mathbb{R}^n$. Let us furthermore assume, that Ω is brick shaped, and that its faces are parallel to the coordinate planes. According to [JKO94, WEH02, Tor02, Hor97] the effective thermal conductivity tensor $\widetilde{K}$ of Ω can be deduced by post-processing n solutions $u_i,\ i = 1, \ldots, n$ of

$$\begin{aligned} \nabla \cdot (K \nabla u_i) &= 0, \quad \text{in } \Omega \\ u_i &= x_i, \quad \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where the conductivity $K = K(\boldsymbol{x})$ may vary on a small length-scale, and where x_i is the i-th component of $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$.

The above problem is the starting point of our considerations. Our target is to consider and discuss an efficient approach for solving it in the case when $K = K(\boldsymbol{x})$ and Ω represent

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a fibrous geometry. Typically, fibrous geometries, e.g. glass- or mineral-wool, satisfy the following properties:

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

Let Ω_M and Ω_A be two open sets satisfying some mild regularity assumptions described in [EIL$^+$07], such that $\overline{\Omega}_M \cup \overline{\Omega}_A = \overline{\Omega}$. We think of Ω_M and Ω_A being the highly (metal, glass) and lowly (air) conductive parts of Ω, respectively. Let us for simplicity assume, that

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

where $\delta \ll 1$. Note, that for high contrast media (i.e. whenever $K_A \ll K_M$) we can meet these assumptions by scaling (1) by K_M^{-1}.

With $u_i,\ i = 1, \ldots, n$ solving (1) we obtain the effective conductivity $\widetilde{K}$ by

$$\widetilde{K}\boldsymbol{e}_i = -\left\langle \boldsymbol{\phi}_i \right\rangle_\Omega, \tag{2}$$

where $\boldsymbol{\phi}_i := -K\nabla u_i$ and $\langle\cdot\rangle_\Omega := \dfrac{1}{|\Omega|}\displaystyle\int_\Omega \cdot\, d\boldsymbol{x}$ denotes the volume average over Ω (cf. [WEH02]) and $\boldsymbol{e}_i$ is the i-th unit vector.

In [EIL$^+$07] it was shown, that

$$\widetilde{K}\boldsymbol{e}_i = -\frac{1}{|\Omega|}\int_{\Omega_M} \boldsymbol{\psi}_i + \mathcal{O}(\delta), \quad i = 1, \ldots, n, \tag{3}$$

where $\boldsymbol{\psi}_i$ satisfies

$$\begin{cases} \nabla \cdot \boldsymbol{\psi}_i &= 0 \quad \text{in } \Omega_M \\ \boldsymbol{\psi}_i &= -K\nabla v_i \quad \text{in } \Omega_M \\ \boldsymbol{\psi}_i \cdot \boldsymbol{n} &= 0 \quad \text{on } \partial\Omega_M \backslash \partial\Omega \\ v_i &= x_i \quad \text{on } \partial\Omega \cap \partial\Omega_M, \end{cases} \tag{4}$$

with $\boldsymbol{n}$ denoting the outer unit normal vector. Here we assume, that all path-connected components of Ω_M touch $\partial\Omega$. According to [EIL$^+$07] we may always assume, that this condition is satisfied (otherwise, we disregard those path-connected components of Ω_M that do not touch the boundary).

The aim of this paper is to efficiently approximate the effective thermal conductivity of fibrous structures (cf. Figure 1). Thus, in the setting introduced above Ω_M is the part of Ω occupied by fibers and some binder material discussed in Remark 2.1. In computing the effective thermal conductivity we take advantage of the slender shape of the fibers and solve (4) on the graph induced by the fiber network. In order to do this we present a proper mimetic finite volume discretization of the Laplace equation on the domain occupied by fibers only and carefully analyze the properties of this discretization. Additionally, we compare the performance of the presented approach for calculating effective thermal conductivities of fibrous materials, with the performance of a commercially available software, namely GeoDict[1].

It should be noted that the considered approach of solving only in the highly conductive part of the domain when computing the effective properties of composite materials, is not a new one. Engineers and physicists have applied it for a long time, based on dimensional analysis and on arguments from physics. In this paper we present a careful mathematical discretization, and what is more important, we discuss the mathematical properties of the

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

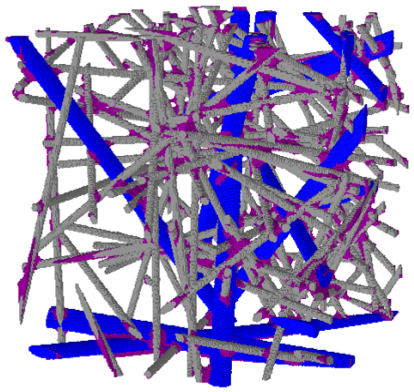


FIGURE 1. 3-dimensional fiber structure with binder material.

derived discretization. In order to give an impression of the engineering and mechanical papers dealing with calculating effective properties of fibrous materials and the like, let us shortly discuss a very old and a very new article. The flow in porous media is described by the same equations as above, and a well known approach for calculating the permeability of fractured porous media suggested by Barenblatt in the 1960s relies on evaluating the flow in the fractures and neglecting the flow through the remaining big but lowly permeable part of the domain. The approach is widely used in geoscience, however, we are not aware of a mathematical study of this approximation.

From the recent considerations, we refer to [VOF$^+$a, VOF$^+$b]. The authors perform a careful dimensional analysis for the cases of perfect, weak, and bad contacts between fibers. In the case of perfect contact, they end with a discretization which is equivalent to the one which will be presented in this paper. However, they do not discuss the properties of the discretized system. It should also be noted that the lowly conductive part of the domain is not considered at all in [BER84] and in [VOF$^+$a, VOF$^+$b]. As we will demonstrate below, accounting for the lowly conductive part of the domain is essential for the correct calculation of the effective thermal conductivities of highly porous materials (e.g. many insulation materials). Below we will show how one can account for the contribution of the lowly conductive part in a cheap way.

It should also be mentioned that fibrous materials and the like are also subject to intensive studies in homogenization theory. The objective there, however, is somehow different from our goal. For example, in [Pan05] Panasenko focuses on the derivation of a homogenized solution living on the skeleton corresponding to a rod structure, as the diameter of the rods tends to zero. Another interesting study is the one in [CJLP02] and [CEJ01] (see also the references therein). In these papers the authors consider periodic lattice structures embedded in some larger domains. On these lattice structures scalar elliptic equations are considered along with Dirichlet boundary conditions on the intersection of the boundaries of the domain and its enclosed lattice structure. On the remaining parts of the boundary of the lattice structure zero Neumann boundary conditions are imposed. Note, that this setting is in fact very similar to (4), i.e. the problem whose solution we would like to approximate efficiently. In [CJLP02] and [CEJ01] the objective is, however, to compute the effective material property of the considered domain as the period of the enclosed lattice structure and the diameter of the involved trusses tend to zero. Thus, as in [Pan05], the objectives in [CJLP02] and [CEJ01] are analytical statements about the convergence of the

fine scale to some homogenized solution and the existence and the properties of effective material properties when the period and/or the diameter of the trusses tends to zero.

The works just mentioned as well as other related homogenization studies of fibrous materials differ from our considerations in several aspects. In particular, the focus there is not on the efficient numerical computation of effective material properties. Furthermore, the lowly conductive parts of the domain are usually not discussed, when computing the effective material properties of the entire domain. Unlike the homogenization articles mentioned above, we consider a fixed fibrous geometry, and discuss efficient solution approaches for the cases when the conductivity of the fibers dominates the conductivity of the bulk material. In general, finite element or finite volume discretizations of the cell problems, as well as the properties of the discretized system, are not discussed in the homogenization literature. The latter is the subject of our discussions. Another difference between our study and the articles mentioned above is that they discuss the monodisperse case (i.e. all the fibers have the same diameter). In connection with insulation materials, we are interested in fibrous materials with certain distributions of the fiber diameters, as well as with certain distributions of the lengths of the fibers. The implementation and the numerical experiments are done for the case of a distribution of fiber radii and lengths.

In our setting, the conductivity of the fibers is assumed to be constant (i.e. K_M) and the geometry of the considered fibrous structure is not affected by any limiting process. Considering several highly conductive types of fibers can also be easily done. Our objective is to efficiently compute - for a fixed geometry - an approximation of the solution of (4) and from there an approximation of the effective thermal conductivity tensor of the whole sample Ω based on the assumption, that the contrast between K_A and K_M is rather large.

The remainder of this article is organized as follows: In the next section we introduce some notation and definitions needed for a smooth exposition of our argument. In section 3 we discuss a mimetic finite volume discretization over the graph formed by the fibers. In particular, we show that the presented discretization imposes a symmetric positive definite operator, which justifies the usage of the Conjugate Gradient method. Additionally, a careful analysis of the dependence of the discretization error on the fiber diameters and on the lengths of the graph edges is performed. Section 4 provides some results from numerical simulations demonstrating the accuracy and the efficiency of the presented approach. The last section is devoted to conclusions.

2. Notations and Definitions

In the previous section we mentioned random fibrous geometries as the main target of our considerations. Let us now briefly discuss in some more detail what we mean by this. For a somewhat simpler presentation we restrict our exposition to three spatial dimensions, i.e. $n = 3$, while making some simplifying sketches also in 2 dimensions.

By a fiber we mean a cylindrical object of finite or infinite length. In particular, it is supposed that a fiber has a straight line at its center. Note, that a generalization to curvilinear fibers is straightforward. For each fiber let $\boldsymbol{l}$ be a unit vector pointing into the direction of the line at its center. Furthermore, the length of a fiber is required to be much larger than its diameter. To generate a fibrous geometry these objects are randomly "thrown into" our domain Ω and cut-off at the boundary $\partial\Omega$. Let the set of all intersections of the straight lines at the centers of fibers with $\partial\Omega$ be denoted by $\partial\omega$. The actual numerical generation of our fibrous geometries is done by the GeoDict software. With this random construction different fibers may and in general will intersect.

Now, let ω be the set of points, where two or more fibers cross. For a simpler presentation and to avoid unnecessary technicalities, we assume, that whenever two fibers (i.e. the cylindrical objects) have a nonempty intersection the same holds true for their center lines. We also define $\overline{\omega} := \omega \cup \partial\omega$. Let h be the characteristic distance between adjacent

(i.e. adjacent on a fiber) nodes in $\overline{\omega}$ and let d be the characteristic diameter of all fibers in $\overline{\Omega}$. We require $d \ll h$ in order to have a meaningful notion of a graph induced by the fibers (which correspond to the edges of the graph) and their intersections (which correspond to the nodes of the graph).

The (circular) cross-section of a fiber perpendicular to $\boldsymbol{l}$ and in the middle of two nodes from $\overline{\omega}$ being adjacent on that fiber is denoted by S. For each cross-section S we denote its center by $\boldsymbol{x}_S := \frac{1}{|S|}\int_S \boldsymbol{\xi} dS(\boldsymbol{\xi})$. The set of all $\boldsymbol{x}_S$ on cross sections between two nodes is denoted by $\mathscr{S}$. The set of all $\boldsymbol{x}_S$ on (circular) faces S being located at those fiber-ends which are inside of Ω is denoted by $\partial\mathscr{S}$. Finally, we set $\overline{\mathscr{S}} := \mathscr{S} \cup \partial\mathscr{S}$. For a better understanding of the definitions above we refer to Figure 2.

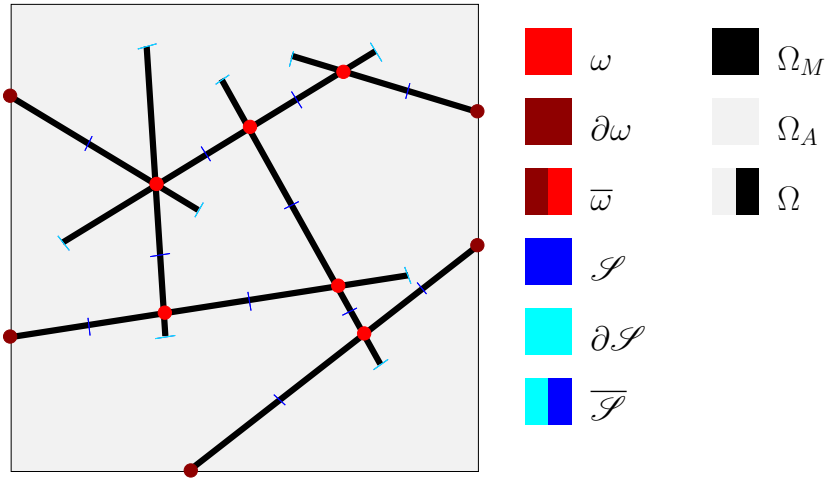


FIGURE 2. Domain with nodes and cross-sections.

For each node $\boldsymbol{x} \in \overline{\omega}$ we define $V_{\boldsymbol{x}}$ to be the volume, which is given by the fiber-segments surrounding $\boldsymbol{x}$ and bounded by the cross-sections S adjacent to $\boldsymbol{x}$. Similarly, for each $S \in \mathscr{S}$ we define V_S to be the cylindrical volume between two adjacent nodes from $\overline{\omega}$, such that S is contained in the enclosed volume (see Figure 3(a)). Note, that near $\boldsymbol{x} \in \omega$ the volumes V_S for different $S \in \mathscr{S}$ actually overlap. These overlapping regions, however, only have a volume, that is $\mathcal{O}(d^n)$. The same estimate holds true for the volumes close to $\boldsymbol{x} \in \partial\omega$, which belong to the fiber but not V_S and vice versa (see Figure 3(b)).

For very regular fiber arrangements depicted in Figures 4(a) (2 dimensional case) and 4(b) (3 dimensional case) it is very easy to see, that

$$\#\overline{\omega} = \mathcal{O}\left(\frac{1}{h^n}\right). \tag{5}$$

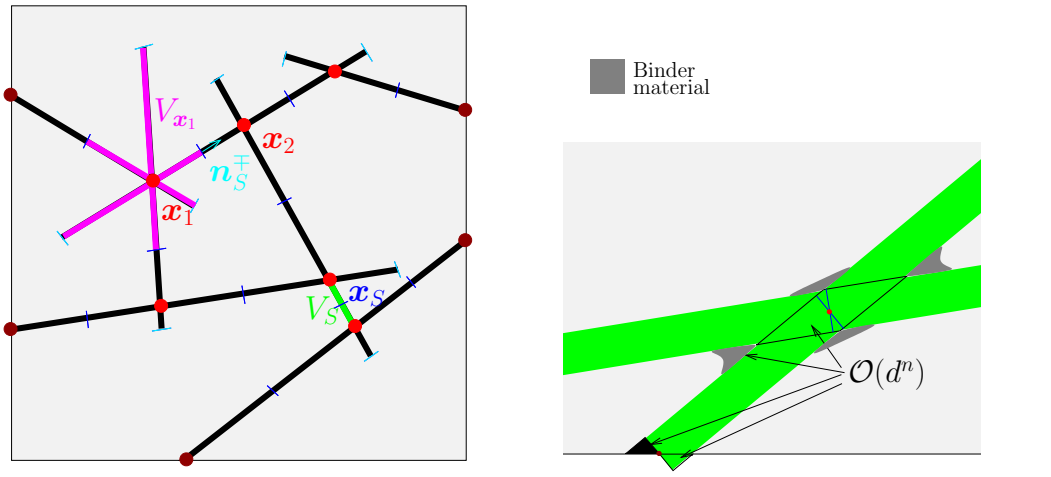
Henceforth, we assume, that estimate (5) also holds true for the fiber geometries, that we consider, which should not be a very restrictive assumption.

Also, we assume that the nodes in $\overline{\omega}$ (and their corresponding surrounding volumes) are numbered, and we define $\boldsymbol{n}_S^{\mp}$ to be the unit normal vector to S pointing from the lower numbered volume to the higher numbered one (see Figure 3).

Remark 2.1. As indicated in section 1 one very often applies some binder material in the production process of glass and mineral wool. For simplicity the thermal conductivity of this binder material is assumed to be equal to that of the fibers. Figures 1 and 3(b) show how this binder can be deposited at the fibers. The volume of each binder segment is

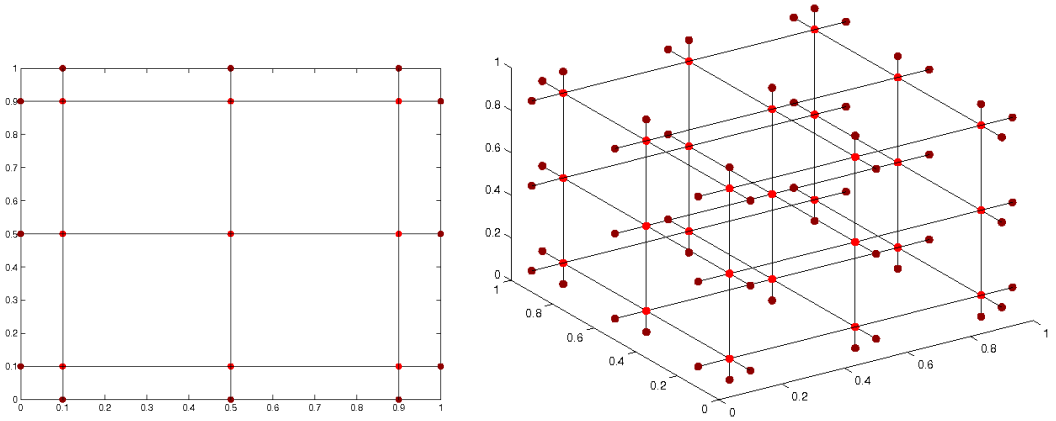
supposed to be $\mathcal{O}(d^n)$, and as for the fiber crossings we expect to have $\mathcal{O}\left(\frac{1}{h^n}\right)$ of these segments.

For the analysis carried out in section 3 it is important to note that due to this binder material we may assume the boundary of Ω_M to have no re-entrant corners. Thus, the solution of (4) has no singularities and is therefore smooth enough for our derivations.



(a) Elementary volumes and normal vectors. (b) Elementary volumes V_S with sections of size $\mathcal{O}(d^n)$.

FIGURE 3. Over-all (a) and zoomed-in (b) sketches of fibrous structures.



(a) 2-D (b) 3-D

FIGURE 4. Interior and boundary nodes for a regular fiber structure.

Now, we define the following spaces of functions being defined on $\overline{\omega}$ and $\overline{\mathscr{S}}$, respectively.

Definition 2.2.

$$\mathscr{U} := \{y : \overline{\omega} \to \mathbb{R}\}, \tag{6a}$$

$$\mathscr{F} := \left\{\boldsymbol{\chi} : \overline{\mathscr{S}} \to \mathbb{R}^3 : \ \boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S = 0 \ \forall \boldsymbol{x}_S \in \partial\mathscr{S}\right\}, \tag{6b}$$

where the $\boldsymbol{n}_S$ are unit vectors being normal to the faces at the ends of the fibers and pointing to the outside of the fibers.

Having defined the quantities and spaces above we are now able to introduce difference operators and scalar products on the unstructured grids given by $\overline{\omega}$ and $\overline{\mathscr{S}}$. We define difference operators $\mathcal{G}$ and $\mathcal{D}$ corresponding to the differential operators ∇ and $\nabla\cdot$, respectively.

Definition 2.3.

$$\begin{aligned} &\mathcal{G} : \mathscr{U} \to \mathscr{F}, \text{ such that} \\ &\mathcal{G}y(\boldsymbol{x}_S) = \frac{y(\boldsymbol{x}_S^+) - y(\boldsymbol{x}_S^-)}{\|\boldsymbol{x}_S^- - \boldsymbol{x}_S^+\|_2}\boldsymbol{n}_S^{\mp} \quad \forall \boldsymbol{x}_S \in \mathscr{S} \\ &\text{and } \mathcal{G}y(\boldsymbol{x}_S) = \boldsymbol{0} \quad \forall \boldsymbol{x}_S \in \partial\mathscr{S}, \end{aligned} \tag{7a}$$

where $\|\cdot\|_2$ denotes the standard Euclidean norm in $\mathbb{R}^n$.

$$\begin{aligned} &\mathcal{D} : \mathscr{F} \to \mathscr{U}, \text{ such that} \\ \mathcal{D}\boldsymbol{\chi}(\boldsymbol{x}) &= \frac{1}{|V_{\boldsymbol{x}}|} \sum_{\substack{S \in \overline{\mathscr{S}} \text{ with} \\ S \subset \partial V_{\boldsymbol{x}}}} \boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S |S|, \quad \forall \boldsymbol{x} \in \overline{\omega} \\ &= \frac{1}{|V_{\boldsymbol{x}}|} \sum_{\substack{S \in \mathscr{S} \text{ with} \\ S \subset \partial V_{\boldsymbol{x}}}} \boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S |S|, \quad \forall \boldsymbol{x} \in \overline{\omega}, \quad \text{since } \boldsymbol{\chi} \cdot \boldsymbol{n}_S|_{\partial\mathscr{S}} = 0. \end{aligned} \tag{7b}$$

Here $\boldsymbol{x}_S^+$ and $\boldsymbol{x}_S^-$ denote the higher and lower numbered node adjacent to S, respectively, and $\boldsymbol{n}_S$ is the unit normal vector to S pointing outside of $V_{\boldsymbol{x}}$.

Furthermore, we define the following scalar products on $\mathscr{U}$ and $\mathscr{F}$.

Definition 2.4.

$$(y, \widetilde{y})_{\mathscr{U}} = \sum_{\boldsymbol{x} \in \overline{\omega}} |V_{\boldsymbol{x}}| y(\boldsymbol{x}) \widetilde{y}(\boldsymbol{x}), \tag{8a}$$

$$(\boldsymbol{\chi}, \widetilde{\boldsymbol{\chi}})_{\mathscr{F}} = \sum_{\boldsymbol{x} \in \overline{\omega}} \sum_{\substack{S \in \mathscr{S} \text{ with} \\ S \subset \partial V_{\boldsymbol{x}}}} |S| dist(\boldsymbol{x}, S) (\boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S)(\widetilde{\boldsymbol{\chi}}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S). \tag{8b}$$

As usual, we denote the norms induced by these scalar products by $\|\cdot\|_{\mathscr{U}}$ and $\|\cdot\|_{\mathscr{F}}$, respectively.

3. Discretization of the Problem and Error Estimates

We first state an important property of the difference operators $\mathcal{G}$ and $\mathcal{D}$, which corresponds to the fact that $\nabla = -\nabla\cdot^*$ for suitable function spaces (here * denotes the adjoint w.r.t. the L^2-inner-product).

Lemma 3.1. *With the definitions and notations above we have, that for all $y \in \mathscr{U}$ and $\boldsymbol{\chi} \in \mathscr{F}$*

$$(y, \mathcal{D}\boldsymbol{\chi})_{\mathscr{U}} = -\left(\mathcal{G}y, \boldsymbol{\chi}\right)_{\mathscr{F}}. \tag{9}$$

Proof. Observe, that

$$\begin{aligned} (y, \mathcal{D}\boldsymbol{\chi})_{\mathscr{U}} &= \sum_{\boldsymbol{x} \in \overline{\omega}} |V_{\boldsymbol{x}}| y(\boldsymbol{x}) \frac{1}{|V_{\boldsymbol{x}}|} \sum_{\substack{S \in \mathscr{S} \text{ with} \\ S \subset \partial V_{\boldsymbol{x}}}} \boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S |S| \\ &= \sum_{\boldsymbol{x} \in \overline{\omega}} \sum_{\substack{S \in \mathscr{S} \text{ with} \\ S \subset \partial V_{\boldsymbol{x}}}} y(\boldsymbol{x}) \boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S |S| \\ &= \sum_{S \in \mathscr{S}} \boldsymbol{\chi}(\boldsymbol{x}_S) \cdot \boldsymbol{n}_S^{\mp} \left(y(\boldsymbol{x}_S^-) - y(\boldsymbol{x}_S^+)\right) |S|, \end{aligned} \tag{10}$$

where the last equality follows from the fact, that each $S \in \mathscr{S}$ is summed over exactly twice (once for each node on either side of S). On the other hand we have

(11)

$$\begin{aligned} -(\mathcal{G}y, \boldsymbol{\chi})_{\mathscr{F}} &= -\sum_{\boldsymbol{x}\in\overline{\omega}} \sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} |S| dist(\boldsymbol{x}, S) \left(\boldsymbol{\chi}(\boldsymbol{x}_S)\cdot\boldsymbol{n}_S\right) \left(\frac{y(\boldsymbol{x}_S^+) - y(\boldsymbol{x}_S^-)}{\|\boldsymbol{x}_S^- - \boldsymbol{x}_S^+\|_2} \boldsymbol{n}_S^{\mp}\cdot\boldsymbol{n}_S\right) \\ &= -\sum_{\boldsymbol{x}\in\overline{\omega}} \sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} |S| \frac{1}{2} \left(\boldsymbol{\chi}(\boldsymbol{x}_S)\cdot\boldsymbol{n}_S\right) \boldsymbol{n}_S\cdot\boldsymbol{n}_S^{\mp} \left(y(\boldsymbol{x}_S^+) - y(\boldsymbol{x}_S^-)\right) \\ &= \sum_{\boldsymbol{x}\in\overline{\omega}} \sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} |S| \frac{1}{2} \left(\boldsymbol{\chi}(\boldsymbol{x}_S)\cdot\boldsymbol{n}_S^{\mp}\right) \left(y(\boldsymbol{x}_S^-) - y(\boldsymbol{x}_S^+)\right) \\ &= \sum_{S\in\mathscr{S}} \boldsymbol{\chi}(\boldsymbol{x}_S)\cdot\boldsymbol{n}_S^{\mp} \left(y(\boldsymbol{x}_S^-) - y(\boldsymbol{x}_S^+)\right) |S|, \end{aligned}$$

where to obtain the second equality we have used that $dist(\boldsymbol{x}_S^-, S) = dist(\boldsymbol{x}_S^+, S) = \frac{1}{2}\|\boldsymbol{x}_S^- - \boldsymbol{x}_S^+\|_2$, which holds by construction. The last equality follows by a similar observation.

Combining (10) and (11) we obtain our claim. □

We now prove a discrete Poincaré type inequality. For this we need the following

Definition 3.2. Let $y \in \mathscr{U}$ then

$$\|y\|_{\mathcal{G}}^2 := (\mathcal{G}y, \mathcal{G}y)_{\mathscr{F}} + (y, y)_{\mathscr{U}} \tag{12a}$$

and

$$|y|_{\mathcal{G}}^2 := (\mathcal{G}y, \mathcal{G}y)_{\mathscr{F}}\,. \tag{12b}$$

It is easy to see, that $\|\cdot\|_{\mathcal{G}}$ and $|\cdot|_{\mathcal{G}}$ define a norm and a semi-norm on $\mathscr{U}$, respectively. Like for other Poincaré type inequalities we now show, that on a suitable subspace of $\mathscr{U}$, $\|\cdot\|_{\mathcal{G}}$ and $|\cdot|_{\mathcal{G}}$ are actually equivalent norms.

Proposition 3.3. *Let $y \in \mathscr{U}$ such that $y|_{\partial\omega} \equiv 0$, then $\exists C$, such that*

$$\|y\|_{\mathcal{G}}^2 \leq C|y|_{\mathcal{G}}^2, \tag{13}$$

where C is a generic constant independent of y.

Proof. Suppose the statement were wrong. Then $\forall C\ \exists y \in \mathscr{U}$ with $y|_{\partial\omega} \equiv 0$ such that $\|y\|_{\mathcal{G}}^2 > C|y|_{\mathcal{G}}^2$. In particular:

$$\forall m \in \mathbb{N}\ \exists y_m \text{ such that } \|y_m\|_{\mathcal{G}}^2 > m|y_m|_{\mathcal{G}}^2.$$

Devision by $\|y_m\|_{\mathcal{G}}^2$ yields:

$$\frac{1}{m} > |\widetilde{y}_m|_{\mathcal{G}}^2,$$

where $\widetilde{y}_m := \dfrac{y_m}{\|y_m\|_{\mathcal{G}}}$ and thus $\|\widetilde{y}_m\|_{\mathcal{G}} = 1$.

Since $(\mathscr{U}, \|\cdot\|_{\mathcal{G}})$ is a finite dimensional normed vector space, and since $\{\widetilde{y}_m\}_{m\in\mathbb{N}}$ is a bounded sequence, we know that there exists a subsequence - again denoted by $\{\widetilde{y}_m\}$ - that converges to, say, $\widetilde{y} \in \mathscr{U}$. We certainly have, that

$$\|\widetilde{y}\|_{\mathcal{G}} = 1 \text{ and } (\mathcal{G}\widetilde{y}, \mathcal{G}\widetilde{y})_{\mathscr{F}} = |\widetilde{y}|_{\mathcal{G}}^2 = 0.$$

Using the latter relation and plugging in the definitions of $(\cdot,\cdot)_{\mathscr{F}}$ and $\mathcal{G}\widetilde{y}$ we readily deduce

$$\sum_{S\in\mathscr{S}} |S| \frac{1}{\|\boldsymbol{x}_S^+ - \boldsymbol{x}_S^-\|_2} (\widetilde{y}(\boldsymbol{x}_S^+) - \widetilde{y}(\boldsymbol{x}_S^-))^2 = 0.$$

Thus, $\widetilde{y}(\boldsymbol{x}_S^+) = \widetilde{y}(\boldsymbol{x}_S^-)$ for all $S \in \mathscr{S}$, which implies that $\widetilde{y}$ is piecewise constant (constant on each subset of $\overline{\omega}$ corresponding to a connected component of Ω_M). Since, however, $\widetilde{y}|_{\partial\omega} \equiv 0$ we thus know that $\widetilde{y} \equiv 0$ in $\overline{\omega}$ (each connected component of Ω_M touches $\partial\Omega$ by assumption). This contradicts the fact that $\|\widetilde{y}_m\|_{\mathcal{G}} = 1$, and we have proven our claim. □

With Lemma 3.1 and Proposition 3.3 we have two essential tools for proving the following error estimate in $\|\cdot\|_{\mathcal{G}}$-norm.

Proposition 3.4. *For $i = 1, \ldots, 3$ let $v_i \in H^1(\Omega_M)$ be the solution of*

$$\left\{\begin{array}{rcl} \nabla \cdot \boldsymbol{\psi}_i &=& -f \quad \text{in } \Omega_M \\ \boldsymbol{\psi}_i &=& -K\nabla v_i \quad \text{in } \Omega_M \\ \boldsymbol{\psi}_i \cdot \boldsymbol{n}_{\Omega_M} &=& 0 \quad \text{on } \partial\Omega_M \backslash \partial\Omega \\ v_i &=& x_i \quad \text{on } \partial\Omega \cap \partial\Omega_M, \end{array}\right. \tag{14}$$

where $f \in L^2(\Omega_M)$, and let $y_i \in \mathscr{U}$ be the solution of

$$\begin{array}{rcl} \mathcal{D}(K\mathcal{G}y_i) &=& \widetilde{f} \quad \text{in } \omega \\ y_i &=& x_i \quad \text{on } \partial\omega, \end{array} \tag{15}$$

where $\widetilde{f}(\boldsymbol{x}) := \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\int_{V_{\boldsymbol{x}}} f(\boldsymbol{\xi})d\boldsymbol{\xi}$, $\forall \boldsymbol{x} \in \omega$. Then

$$\|y_i - u_i\|_{\mathcal{G}} = \mathcal{O}\left((h+d)^2\right). \tag{16}$$

As above, h and d is the characteristic distance between two adjacent nodes and the characteristic fiber diameter, respectively.

Remark 3.5. As mentioned above, the discretization given by (15) corresponds to that used in [VOF$^+$a, VOF$^+$b] for the perfect contace case.

Proof. Recall, that for each $S \in \overline{\mathscr{S}}$ its center-point is defined by $\boldsymbol{x}_S := \dfrac{1}{|S|}\displaystyle\int_S \boldsymbol{\xi} dS(\boldsymbol{\xi})$. For a better readability we will drop the subindex i in this proof. Now, for $\boldsymbol{x} \in \omega$ we observe

$$\begin{array}{rcl} & \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\int_{V_{\boldsymbol{x}}} \nabla \cdot \boldsymbol{\psi}(\boldsymbol{\xi}) d\boldsymbol{\xi} & \\ = & \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} \int_S \boldsymbol{\psi}(\boldsymbol{\xi}) \cdot \boldsymbol{n}_S dS(\boldsymbol{\xi}) & \\ = & \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} \int_S \left(\boldsymbol{\psi}(\boldsymbol{x}_S) + \nabla\boldsymbol{\psi}(\boldsymbol{x}_S)\cdot(\boldsymbol{\xi}-\boldsymbol{x}_S) + \mathcal{O}(|\boldsymbol{\xi}-\boldsymbol{x}_S|^2)\right)\cdot \boldsymbol{n}_S dS(\boldsymbol{\xi}) & (17) \\ = & \mathcal{D}\boldsymbol{\psi}(\boldsymbol{x}) + \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} \Big(\nabla\boldsymbol{\psi}(\boldsymbol{x}_S)\cdot \underbrace{\int_S \boldsymbol{\xi}-\boldsymbol{x}_S dS(\boldsymbol{\xi})}_{=|S|\boldsymbol{x}_S - |S|\boldsymbol{x}_S = 0}\cdot \boldsymbol{n}_S + \int_S \mathcal{O}(d^2)\cdot\boldsymbol{n}_S dS(\boldsymbol{\xi})\Big) & \\ = & \mathcal{D}\boldsymbol{\psi}(\boldsymbol{x}) + \mathcal{D}\left(\mathcal{O}(d^2)\right). & \end{array}$$

Secondly, we observe, that

$$\begin{array}{rcl} \mathcal{D}(K\mathcal{G}v)(\boldsymbol{x}) &=& \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} \frac{v(\boldsymbol{x}_S^+) - v(\boldsymbol{x}_S^-)}{\|\boldsymbol{x}_S^- - \boldsymbol{x}_S^+\|_2}\boldsymbol{n}_S^{\mp}\cdot\boldsymbol{n}_S|S|K(\boldsymbol{x}_S) \\ &=& \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} \left(\nabla v(\boldsymbol{x}_S)\cdot\boldsymbol{n}_S^{\mp} + \mathcal{O}(dist(S,\boldsymbol{x}_S^-)^2)\boldsymbol{n}_S^{\mp}\right)\cdot\boldsymbol{n}_S|S|K_M \\ &=& -\mathcal{D}\boldsymbol{\psi}(\boldsymbol{x}) + \dfrac{1}{|V_{\boldsymbol{x}}|}\displaystyle\sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} \mathcal{O}(h^2)\cdot\boldsymbol{n}_S|S| \\ &=& -\mathcal{D}\boldsymbol{\psi}(\boldsymbol{x}) + \mathcal{D}\left(\mathcal{O}(h^2)\right), \end{array} \tag{18}$$

where we have used Taylor expansion and the fact that $dist(S, \boldsymbol{x}_S^-) = dist(S, \boldsymbol{x}_S^+) = \frac{1}{2}\|\boldsymbol{x}_S^- - \boldsymbol{x}_S^+\|_2$.

Combining (17) and (18) we thus obtain

$$\mathcal{D}(K\mathcal{G}v)(\boldsymbol{x}) = -\frac{1}{|V_{\boldsymbol{x}}|}\int_{V_{\boldsymbol{x}}} \nabla\cdot\boldsymbol{\psi}(\boldsymbol{\xi})d\boldsymbol{\xi} + \mathcal{D}\left(\mathcal{O}(h^2)\right) + \mathcal{D}\left(\mathcal{O}(d^2)\right). \tag{19}$$

Now, since $\nabla\cdot\boldsymbol{\psi} = -f$ we obtain by the definition of $\widetilde{f}$ that

$$\mathcal{D}(K\mathcal{G}v)(\boldsymbol{x}) = \widetilde{f}(\boldsymbol{x}) + \mathcal{D}\left(\mathcal{O}(h^2)\right) + \mathcal{D}\left(\mathcal{O}(d^2)\right). \tag{20}$$

Due to (15) we are therefore left with

$$\mathcal{D}\left(K\mathcal{G}(v-y)\right)(\boldsymbol{x}) = \mathcal{D}\left(\mathcal{O}(d^2)\right) + \mathcal{D}\left(\mathcal{O}(h)^2\right). \tag{21}$$

Multiplying (21) scalarly by $v-y$ yields

(22)
$$\begin{array}{rrcl} & (\mathcal{D}(K\mathcal{G}(v-y)), v-y)_{\mathscr{U}} &=& \left(\mathcal{D}\left(\mathcal{O}(d^2)\right), v-y\right)_{\mathscr{U}} + \left(\mathcal{D}\left(\mathcal{O}(h^2)\right), v-y\right)_{\mathscr{U}} \\ \Rightarrow & K_M\left(\mathcal{G}(v-y), \mathcal{G}(v-y)\right)_{\mathscr{F}} &\leq& \left|\left(\mathcal{O}(d^2), \mathcal{G}(v-y)\right)_{\mathscr{F}}\right| + \left|\left(\mathcal{O}(h^2), \mathcal{G}\left(v-y\right)\right)_{\mathscr{F}}\right| \\ & &\leq& \|\mathcal{G}(v-y)\|_{\mathscr{F}}\left(\left\|\mathcal{O}(d^2)\right\|_{\mathscr{F}} + \left\|\mathcal{O}\left(h^2\right)\right\|_{\mathscr{F}}\right) \\ \Rightarrow & \|v-y\|_{\mathcal{G}} &\leq& \frac{C}{K_M}\left(\|\mathcal{O}(d^2)\|_{\mathscr{F}} + \|\mathcal{O}\left(h^2\right)\|_{\mathscr{F}}\right), \end{array}$$

where we have applied Lemma 3.1, the Cauchy-Schwarz inequality, and Proposition 3.3.

From (22) we easily conclude (16). □

With Proposition 3.4 we are now finally able to state our main result.

Theorem 3.6. *Let $y_i,\ i = 1, \ldots, 3$ be a solution of*

$$\begin{array}{rcll} \mathcal{D}\left(K\mathcal{G}y_i\right) &=& 0 & \text{in } \omega \\ y_i &=& x_i & \text{on } \partial\omega, \end{array} \tag{23}$$

then

$$\widetilde{K}\boldsymbol{e}_i = \frac{1}{|\Omega|}\sum_{S\in\overline{\mathscr{T}}} K_M\mathcal{G}y_i(\boldsymbol{x}_S)|V_S| + \mathcal{O}\left((h+d)^2\right) + \mathcal{O}(\delta) + \mathcal{O}\left(\left(\frac{d}{h}\right)^3\right). \tag{24}$$

Proof. Note, that we have the following:

(25)
$$\begin{aligned} &\left\|\widetilde{K}\boldsymbol{e}_i - \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}} K_M\mathcal{G}y_i(\boldsymbol{x}_S)|V_S|\right\|_2 \\ &= \left\|\frac{-1}{|\Omega|}\int_{\Omega_M}\boldsymbol{\psi}_i d\boldsymbol{x} - \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}} K_M\mathcal{G}y_i(\boldsymbol{x}_S)|V_S|\right\|_2 + \mathcal{O}(\delta) && \text{(by (3))} \\ &= \frac{K_M}{|\Omega|}\left\|\int_{\Omega_M}\nabla v_i d\boldsymbol{x} - \sum_{S\in\mathscr{S}}\mathcal{G}y_i(\boldsymbol{x}_S)|V_S|\right\|_2 + \mathcal{O}(\delta) \\ &= \frac{1}{|\Omega|}\left\|\sum_{S\in\mathscr{S}}\left(\int_{V_S}\nabla v_i d\boldsymbol{x} - \mathcal{G}y_i(\boldsymbol{x}_S)|V_S|\right)\right\|_2 + \mathcal{O}(\delta) + \mathcal{O}\left(\left(\frac{d}{h}\right)^3\right) && \text{(by (5))} \\ &\leq \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}}\left\|\left(\nabla v_i(\boldsymbol{x}_S) + \mathcal{O}(h^2) + \mathcal{O}(d^2)\right)|V_S| - \mathcal{G}y_i(\boldsymbol{x}_S)|V_S|\right\|_2 + \mathcal{O}(\delta) + \mathcal{O}\left(\left(\frac{d}{h}\right)^3\right), \end{aligned}$$

where for the third equality we have used the boundedness (in L^2-norm) of ∇v_i (cf. [EIL+07, Lemma 3.1]) and the fact that the volume of the overlapping and binder regions

depicted in Figure 3(b) is $\mathcal{O}\left(\left(\frac{d}{h}\right)^3\right)$. Now, observe, that $\nabla v_i(\boldsymbol{x}_S) = \frac{v_i(\boldsymbol{x}_S^+) - v_i(\boldsymbol{x}_S^-)}{\|\boldsymbol{x}_S^+ - \boldsymbol{x}_S^-\|_2}\boldsymbol{n}_S^{\mp} + \mathcal{O}(d^2)$. This holds, since every component of $\nabla v_i(\boldsymbol{x}_S)$ normal to $\boldsymbol{n}_S$ is $\mathcal{O}(d^2)$, which in turn follows from the zero Neumann boundary conditions formulated in (4) and the fact, that $\boldsymbol{x}_S$ is in the center of S, i.e. $\boldsymbol{x}_S := \frac{1}{|S|}\int_S \boldsymbol{\xi} dS(\boldsymbol{\xi})$.

With this, and by taking into account the definition of $\mathcal{G}$ we may write

$$
\begin{aligned}
&\left\| \widetilde{K}\boldsymbol{e}_i - \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}} K_M \mathcal{G} y_i(\boldsymbol{x}_S)|V_S| \right\|_2 \\
&\leq \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}} \left\| \mathcal{G}(v_i - y_i)(\boldsymbol{x}_S) + \mathcal{O}(d^2) + \mathcal{O}(h^2) \right\|_2 |V_S| + \mathcal{O}(\delta) + \mathcal{O}\left(\left(\frac{d}{h}\right)^3\right) \qquad (26)\\
&= \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}} \left| \boldsymbol{n}_S \cdot \mathcal{G}(v_i - y_i)(\boldsymbol{x}_S) + \mathcal{O}(d^2) + \mathcal{O}(h^2) \right| |V_S| + \mathcal{O}(\delta) + \mathcal{O}\left(\left(\frac{d}{h}\right)^3\right)
\end{aligned}
$$

Observe, that we have

$$
\begin{aligned}
(\mathcal{G}(v_i - y_i), \mathcal{G}(v_i - y_i))_{\mathscr{F}} &= \sum_{\boldsymbol{x}\in\overline{\omega}} \sum_{\substack{S\in\mathscr{S} \text{ with} \\ S\subset\partial V_{\boldsymbol{x}}}} |S| dist(\boldsymbol{x}, S) \left(\mathcal{G}(v_i - y_i)\cdot\boldsymbol{n}_S\right)\left(\mathcal{G}(v_i - y_i)\cdot\boldsymbol{n}_S\right) \qquad (27)\\
&= \sum_{S\in\mathscr{S}} |V_S| \left(\mathcal{G}(v_i - y_i)(\boldsymbol{x}_S)\cdot\boldsymbol{n}_S\right)^2
\end{aligned}
$$

Combining (26) with (27) and Proposition 3.4 we easily deduce

$$
\left\| \widetilde{K}\boldsymbol{e}_i - \frac{1}{|\Omega|}\sum_{S\in\mathscr{S}} K_M \mathcal{G} y_i(\boldsymbol{x}_S)|V_S| \right\|_2 \leq \mathcal{O}((h+d)^2) + \mathcal{O}(\delta) + \mathcal{O}\left(\left(\frac{d}{h}\right)^3\right),
$$

which clearly implies (24). □

4. Numerical Results

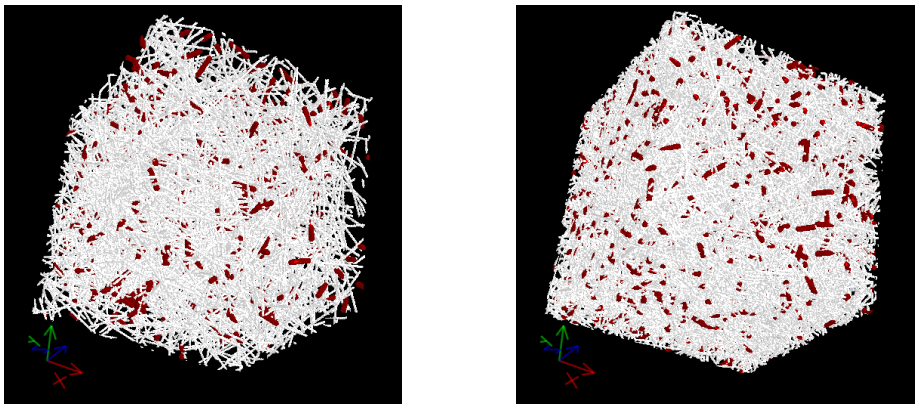
Before taking a look at the numerical results, which can be obtained by applying the theory developed above, let us specify the components of the used algorithm more precisely:

First of all, an analysis is carried out determining all crossings of fibers. (An efficient way of doing this is the content of a forthcoming paper.) Based on this information an undirected graph is constructed. Corresponding to this graph we set up the discrete system defined by (23). The arising linear system is then solved by the ILU preconditioned Conjugate Gradient solver implemented in the LASPack package[2]. Once the solution is obtained, it is post-processed according to (24) to approximate the effective thermal conductivity.

Additionally, we note that as discussed in [EIL+07, section 4] an approximation of the flux in Ω_A and in the path-connected components of Ω_M which don't touch $\partial\Omega$ does enter our computations. Asymptotically, as $\delta \to 0$ these components can be neglected. 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, by taking into account some approximation of the flux in those regions. In the numerical examples presented below 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 the path-connected components of Ω_M not touching the boundary is obtained in the same way and then scaled by δ.

[2]For more details about this package please refer to www.mgnet.org/mgnet/Codes/laspack/html/laspack.html

Now, let us have a look at two specific examples. Both fiber structures are cubic and have a solid volume fraction of 5% (see Figure 5(a)) and 15% (see Figure 5(b)), respectively. In both cases 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). Both fiber geometries are isotropic. They were generated by the GeoDict software using a 500^3 voxel mesh for discretization.



(a) Fiber structure with 5% fibers. (b) Fiber structure with 15% fibers.

FIGURE 5. Two fiber structures with different densities of fibers.

Now, we compare the effective thermal conductivity tensors of these two structures computed by GeoDict, which in turn uses the solver "EJ-HEAT", and by our algorithm described above. In this context we would like to point out, that GeoDict uses periodic boundary conditions in the formulation of the cell problems, whereas we use linear boundary conditions. It is well known (cf. e.g. [BP04]), that for REVs these different types of boundary conditions produce (asymptotically with the length scale of the microscopic variations going to zero) the same effective conductivity tensors. In our examples we consider the case, that the conductivity of the fibers is 50-times larger than the conductivity of the air. By the numerical analysis performed in [IRW07] it is reasonable to assume, that for this contrast both fiber geometries constitute REVs. Also, a contrast of 1:50 corresponds to an application in engineering, namely the conductivities of air and glass or mineral fibers used in glass- and mineral-wool, respectively. Tables 1(a) and 1(b) show the numerical results produced by GeoDict and our algorithm, which we refer to as "COGraph" for both fiber structures, respectively. As stopping tolerance we used $1e-6$ in all cases. For comparing the efficiency, we also report the total runtime of each algorithm and the amount of memory used. Since the off-diagonal elements of the effective thermal conductivity tensors are negligibly small, we only report the diagonal entries. For an objective comparison all computations were performed on the same computer platform.

5. Conclusions

As we can see from the numerical data provided in Table 1, the results produced by COGraph are very much comparable to those of GeoDict - up to two digits they are almost identical. Comparing the required runtime and the used memory, however, we see, that COGraph uses significantly fewer resources. For the geometry containing only 5% fiber material it requires less than 0.02% of the time and about 0.4% of the memory that is

(a) Effective thermal conductivity tensor of the fiber structure shown in 5(a).

	GeoDict			COGraph		
$\widetilde{K}=$	**1.653**	-	-	**1.672**	-	-
	-	**1.637**	-	-	**1.643**	-
	-	-	**1.614**	-	-	**1.624**
# unknowns		1.25e8			3859	
runtime		$>$ 5500sec.			$<$ 1sec.	
memory		3169MB			13MB	

(b) Effective thermal conductivity tensor of the fiber structure shown in 5(b).

	GeoDict			COGraph		
$\widetilde{K}=$	**3.244**	-	-	**3.158**	-	-
	-	**3.190**	-	-	**3.094**	-
	-	-	**3.274**	-	-	**3.205**
# unknowns		1.25e8			26549	
runtime		$>$ 6000sec.			$<$ 5sec.	
memory		4876MB			84MB	

TABLE 1. Comparison of the effective thermal conductivity tensors for the fiber structures shown in Figure 5 computed by GeoDict and COGraph. $K_M = 50$ and $K_A = 1$.

required by the EJ-HEAT solver. For the denser fiber geometry these differences aren't quite as large, however, they remain substantial.

It is obvious, that by increasing the number of fibers, while keeping the size and resolution of the voxelized gird constant, affects the performance of COGraph more than that of GeoDict. The reason is, that usually more fibers have more intersections entailing a higher number of unknowns for COGraph, while the number of unknowns for EJ-HEAT stays exactly the same. Nonetheless, the number of unknowns for COGraph remains several orders of magnitude smaller than that of EJ-HEAT.

These observations also concern a related issue. For geometries where only (very) small fractions of the total volume are occupied by fibers we typically need a (very) large sample size to obtain an REV (cf. [IRW07]). For some glass-/mineral-wool fabrics the solid-volume-fraction is less than 1%. In order to resolve the fibers in such a structure and at the same time consider a large enough sample, one easily needs to consider voxel discretizations with 1000^3, 2000^3, or even more unknowns depending on the remaining material parameters, such as fiber thickness, conductivity of the fiber material, etc. Obviously, there is no chance to solve cell problems on such extremely large grids with standard methods. COGraph, on the other hand, is only sensitive to the number of fiber intersections, which is strongly related to the total number of fibers and thus to the total amount of fiber material in a sample. Due to this property COGraph is, in fact, particularly well suited for calculating the effective thermal conductivity tensors for large sparse fiber geometries.

On the whole, we may say, that our developed algorithm is a specialized tool for computing the effective thermal conductivity tensors of fiber geometries, which exhibit a large contrast between the conductivities of the fiber materials and the surrounding air. For fiber structures with a (very) low solid-volume-fraction it allows to consider (very) large sample sizes, which are too large to be treated by classical methods.

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