ROBUSTNESS OF FINITE ELEMENT SIMULATIONS IN DENSELY PACKED RANDOM PARTICLE COMPOSITES

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Abstract. This paper presents some weighted $H^2$-regularity estimates for a model Poisson problem with discontinuous coefficient at high contrast. The coefficient represents a random particle reinforced composite material, i.e., perfectly conducting circular particles are randomly distributed in some background material with low conductivity. Based on these regularity results we study the percolation of thermal conductivity of the material as the volume fraction of the particles is close to the jammed state. We prove that the characteristic percolation behavior of the material is well captured by standard conforming finite element models.

1. Introduction. This note studies the numerical approximability of thermal diffusion in a representative class of particle composite materials (or composites). The particles (or inclusions) are pairwise disjoint closed disks $I = \{I_1, I_2, \ldots, I_N\}$ with positive radii. They are randomly distributed in a background material (or matrix) that occupies some open, bounded, convex, polygonal domain $\Omega \subset \mathbb{R}^2$. The inclusions are highly conducting compared to the matrix $\Omega_{\text{mat}} := \Omega \setminus \cup I$, a fact which is reflected in the diffusion coefficient

$$c(x) = \begin{cases} 
1 & \text{if } x \in \Omega_{\text{mat}}, \\
\text{c}_{\text{cont}} & \text{if } x \in \cup I
\end{cases}$$

with some contrast parameter $c_{\text{cont}} \gg 1$.

The thermal diffusion in the composite is modeled by the stationary heat equation,

$$-\text{div} \ c \nabla u = f \text{ in } \Omega, \quad u = u_D \text{ on } \partial \Omega,$$

with a prescribed temperature $u_D$ at the boundary of $\Omega$ and a heat source $f$. If the source term $f$ is supported in the matrix and if the inclusions are assumed to be perfectly conducting ($c_{\text{cont}} = \infty$), then problem (2) reduces to an equation in the perforated domain $\Omega_{\text{mat}}$. Consider the function spaces

$$V := \{v \in H^1(\Omega_{\text{mat}}) : v|_{\partial I} = \text{const. for all } I \in I\}$$

and

$$V_0 := \{v \in V : v|_{\partial \Omega} = 0 \text{ in the sense of traces}\}.$$


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Then the corresponding variational problem reads: Given $f \in L^2(\Omega^{\text{mat}})$ and $u_D \in C^2(\partial \Omega)$, find $u \in V$ such that

$$
\int_{\Omega^{\text{mat}}} \nabla u(x) \nabla v(x) \, dx = \int_{\Omega^{\text{mat}}} f(x) v(x) \, dx \quad \text{for all } v \in V_0 \quad (3.a)
$$

and

$$
u(x) = u_D(x) \quad \text{for almost all } x \in \partial \Omega. \quad (3.b)
$$

Since the elements of $V$ have a constant trace on the boundary of a single inclusion, they can trivially be extended to $\Omega$ in a way that the extension $v \in H^1(\Omega)$ satisfies $\nabla v|_{(\Omega \setminus I)} \equiv 0$. Hence, the inequalities of Friedrichs and Schwarz yield

$$
\|v\|_{H^1(\Omega^{\text{mat}})} \leq (1 + \text{diam}(\Omega)^2) \|\nabla v\|_{L^2(\Omega^{\text{mat}})} \quad \text{and} \quad (4.a)
$$

$$
\int_{\Omega^{\text{mat}}} \nabla u(x) \nabla v(x) \, dx \leq \|u\|_{H^1(\Omega^{\text{mat}})} \|v\|_{H^1(\Omega^{\text{mat}})} \quad (4.b)
$$

for all $u, v \in V_0$. The inequalities (4) ensure the unique solvability of the variational problem (3).

The major difficulty in discretizing (3) arises from the fact that the energy of the solution $u$, given by $\|\nabla u\|_{L^2(\Omega^{\text{mat}})}^2$, might depend crucially on the geometric properties of the filler. Consider the appearance of an almost conducting path of inclusions, which connects two parts of the outer boundary $\partial \Omega$ where different temperatures are prescribed (as in Figure 1.a). The gap in the temperature needs to be compensated on the path, i.e., in the small regions (characterized by a small parameter $\delta_{\text{cond}}$ in Figure 1.a) between the inclusions of the path. Hence, the solution shows steep gradients there. If the inclusions of the path touch pairwise, the path is perfectly conducting and hence, the energy is infinite. Depending on the volume fraction of particles, the material shows a phase transition from moderate to high conductivity. Mathematically speaking, the solution operator, which maps a pair $(u_D, f) \in C^2(\partial \Omega) \times L^2(\Omega^{\text{mat}})$ to the solution of (3), is not uniformly bounded with respect to the geometry of the set of inclusions $I$.

In this study, we will show that standard conforming finite element approximations of (3) (denoted by $u^{\text{fem}}$) capture such a percolation phenomenon effectively. More precisely,

$$
\|\nabla (u - u^{\text{fem}})\|_{L^2(\Omega^{\text{mat}})} \leq C \quad (5)
$$

holds with some generic constant $C$ independent of the distance of the particles (see Theorem 4.1). This estimate is true although $\|\nabla u\|$ might blow up as described before. Thus, conforming finite element methods are robust with respect to $\delta_{\text{cond}} \to 0$ and allow meaningful material simulation even in densely packed composites.

The issue of percolation and its numerical traceability in transport problems related to high (infinite) contrast particle composites was previously addressed by discrete network models [4, 2, 3]. A pioneering result [3, Theorem 3.3] is that discrete network models, for equally sized inclusions in the absence of outer forces ($f = 0$), mimic the blow-up of the energy as the volume fraction of the particles is close to the jammed state.

Compared to the analysis in [2, 3], which rests mainly on duality arguments, our analysis is built upon regularity estimates for the solution of (3) in certain weighted

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1A finite element method is called conforming if the corresponding finite element space is contained in $V$. In the present context, conformity shall primarily ensure that the complicated geometry of the composite is resolved exactly – or at least sufficiently accurate compared to the geometric scales in the problem – by the underlying finite element mesh.
norms. In this context, the weight (denoted by $\delta$) reflects the local thickness of the perforated domain $\Omega^{\text{mat}}$ (see Section 2.1). By choosing this specific weight, the constant in the regularity estimates (cf. Theorems 3.3 and 3.5) turns out to be independent of $\delta$, i.e., they do not depend on the distances between the inclusions. The combination of the quasi-optimality of conforming finite elements, standard interpolation error estimates, and the new regularity estimates yield the general statement on robustness (5) without even specifying a discrete space precisely. Our technique generalizes in a straightforward way to problem classes beyond the model problem under consideration, e.g., to more general inclusion geometries, to the 3-dimensional case, and to general second order elliptic operators.

2. Geometric preliminaries. This section manifests the notion of thickness of a perforated domain and a finite, problem-adapted subdivision of the perforated domain under consideration.

2.1. The thickness of a domain. Our definition of thickness relies on a certain (infinite) triangulation of $\Omega^{\text{mat}}$, which is first introduced.

A convex polygon $T$ is the convex hull of 2 or more distinct points. The set of its vertices (corners) $V(T)$ is the minimal set of points $x_1, x_2, \ldots, x_k \in \mathbb{R}^2$, so that $T = \text{conv}\{x_1, x_2, \ldots, x_k\}$. According to the above definition, convex polygons are closed. A convex polygon $T$ is called cyclic if its vertices (corners) $V(T)$ are located on the boundary of its (closed) circumdisk $CD(T)$. Examples of cyclic polygons are line segments, triangles and rectangles.

Following [9], $\Omega^{\text{mat}}$ can be represented by a regular, infinite subdivision $\mathcal{T}_{\text{mat}}$ into cyclic polygons (or triangulation for short). More precisely, $\mathcal{T}_{\text{mat}}$ is a set of cyclic polygons such that its set of vertices $V(\mathcal{T}_{\text{mat}})$ equals $\partial \Omega^{\text{mat}}$, 

$$V(\mathcal{T}_{\text{mat}}) := \bigcup_{T \in \mathcal{T}_{\text{mat}}} V(T) = \partial \Omega^{\text{mat}},$$

and any two distinct cyclic polygons in $\mathcal{T}_{\text{mat}}$ are either disjoint, or share exactly one vertex, or have exactly one edge in common. Moreover, the triangulation $\mathcal{T}_{\text{mat}}$ can be chosen in a way that all of its elements $T \in \mathcal{T}_{\text{mat}}$ satisfy the so-called Delaunay criterion

$$CD(T) \cap V(\mathcal{T}_{\text{mat}}) = V(T). \tag{6}$$

Figure 1.b depicts $\mathcal{T}_{\text{mat}}$ for some set of inclusions (the thick edges between neighboring inclusions are unions of line segments to be explained in Section 2.2; see Figure 2 for a zoom).

Remark 1. The elements of the Delaunay triangulation $\mathcal{T}_{\text{mat}}$ can be characterized locally: Let $x \in \partial \Omega^{\text{mat}}$ be any point on the boundary of $\Omega^{\text{mat}}$ and $\nu_x$ be the corresponding outer normal vector, let $A$ be some closed subset of $\partial \Omega^{\text{mat}}$, and let

$$\Pi(x, A) := \arg\min_{y \in A} \max\{\text{dist}(x, y), 0\} \neq \emptyset \tag{7}$$

be the set of points in $A$ which are closest to $x$ in normal direction. Then the cyclic polygon $T_x := \text{conv}(x \cup \Pi(x, \partial \Omega^{\text{mat}})) \in \mathcal{T}_{\text{mat}}$. Moreover, for all $T \in \mathcal{T}_{\text{mat}}$ there is some $x \in \partial \Omega^{\text{mat}}$ such that $T = T_x$.

Since the Delaunay criterion (6) ensures that $\text{int}(CD(T)) \subset \Omega^{\text{mat}}$ for all $T \in \mathcal{T}_{\text{mat}}$, the diameter of $T$ may serve as a local measure of the thickness of the perforated domain $\Omega^{\text{mat}}$. 

Definition 2.1 (Thickness of a domain). The $\mathcal{T}_{\text{mat}}$-piecewise constant function $\delta : \Omega^{\text{mat}} \to \mathbb{R}_{>0}$, given by
$$
\delta|_T := \delta_T := \text{diam}(\text{CD}(T)) \quad \text{for } T \in \mathcal{T}_{\text{mat}},
$$
is denoted as the thickness of $\Omega^{\text{mat}}$.

2.2. A finite subdivision of perforated domains. Inspired by [2], a finite subdivision of the perforated $\Omega^{\text{mat}}$ is extracted from the infinite triangulation $\mathcal{T}_{\text{mat}}$ which was introduced in the previous subsection. Without loss of generality let us make the following technical assumption.

Assumption 2.2. An element of $\mathcal{T}_{\text{mat}}$ shall either be a line segment or a triangle. In addition, every pair of triangles shall be separated by at least one line segment.

Remark 2. Assumption 2.2 is not fulfilled in general. The triangulation $\mathcal{T}_{\text{mat}}$ might contain cyclic polygons with more than three vertices. Their appearance is related to the lack of uniqueness of the Delaunay triangulation (into triangles) if the given points are not in general position\(^2\). However, this degeneracy can be circumvented by subdividing every cyclic polygon with more than three vertices into triangles. The resulting new triangles are not separated by a line segment but share a common edge. This edge can simply be added as an element to the triangulation $\mathcal{T}_{\text{mat}}$.

Let $\mathcal{H} := \{H_1, H_2, \ldots, H_M\}$ be a minimal set of shifted halfspaces that form the outer boundary of $\Omega$, i.e.,
$$
\Omega^c := \mathbb{R}^2 \setminus \Omega = \bigcup_{k=1}^{M} H_k.
$$

---

\(^2\)A set of points in the plane is in general position if no four points lie on a common circle.
Since the halfspaces in the set $\mathcal{H}$ can be regarded as disks with infinite radius we define an extended set of inclusions $\tilde{\mathcal{I}} := \mathcal{I} \cup \mathcal{H}$.

A cyclic polygon $T \in \mathcal{T}_{\text{mat}}$ with vertices $x_1, \ldots, x_k \in \partial \Omega_{\text{mat}}$ ($k = 2$ or $3$) connects a subset of inclusions $\{I_1, \ldots, I_k\} \subset \tilde{\mathcal{I}}$ if it satisfies $x_j \in I_j$ for all $j = 1, \ldots, k$. For any $T \in \mathcal{T}_{\text{mat}}$ let $\tilde{\mathcal{I}}(T)$ denote the maximal set of inclusions that is connected by $T$.

In this respect, $\tilde{\mathcal{I}}(\cdot)$ can be interpreted as a mapping from $\mathcal{T}_{\text{mat}}$ into the power set of $\tilde{\mathcal{I}}$. The desired finite partition of $\Omega_{\text{mat}}$ is given by the quotient modulo of this mapping $\tilde{\mathcal{I}}(\cdot)$. It is denoted as the generalized Delaunay partition $\mathcal{D}$ (see [8, 9]) and consists of curvilinear polygons, more precisely

1. (generalized) edges, i.e., channel-like objects (unions of line segments) that connect two neighboring inclusions, and
2. triangles.

According to the classification above, we distinguish between the set of edges $\mathcal{E} \subset \mathcal{D}$ and the set of triangles $\mathcal{T} = \mathcal{D} \setminus \mathcal{E}$.

We emphasize that the generalized Delaunay triangulation serves as a tool in the subsequent regularity analysis. It is a natural way to represent the geometry of particle reinforced composite materials, but it is not based on physical grounds.

3. Thickness-weighted regularity.

3.1. Preliminary remarks. Recall the classical $H^2$-regularity result on a smooth ($C^2$) domain $K \subset \mathbb{R}^2$ as it is stated in every textbook on partial differential equations (e.g., [6, Theorem 6.4]): Any $u \in H^1_0(K)$ with $\Delta u \in L^2(K)$ is in $H^2(K)$ and there is a constant $C$ that does not depend on $u$ such that

$$\|\nabla^2 u\|_{L^2(K)} \leq C \|\Delta u\|_{L^2(K)}. \quad (8)$$

This result extends to certain domains with piecewise analytic boundary, especially to the elements of the subdivision $\mathcal{D}$ from Section 2.2. In [1], $K$ is considered to be a curvilinear polygon, i.e., $K$ is a simply-connected, bounded domain with the boundary $\partial K = \bigcup_{k=1}^m \Gamma_k$, where $\Gamma_k$ are analytic simple arcs,

$$\tilde{\Gamma}_k = \{\phi_k(\xi) : \xi \in [-1, 1]\}. $$

The functions $\phi_k$ are analytic on $[-1, 1]$ with $|\nabla \phi_k|$ being bounded away from zero. Under the assumption that all internal angles $\gamma_1, \gamma_2, \ldots, \gamma_m$ of $K$ satisfy $0 < \gamma_k \leq \pi$, there is a constant $C_{\text{reg}}$ such that

$$\|\nabla^2 u\|_{L^2(K)} \leq C_{\text{reg}} \|\Delta u\|_{L^2(K)} \quad (9)$$

holds for all $u \in H^1_0(K)$ with $\Delta u \in L^2(K)$. Let us stress that the constant $C_{\text{reg}}$ does not depend on the scaling of $K$ (see, e.g., [7, Remark 5.5.6]).

3.2. Local regularity.

3.2.1. Regularity on generalized edges. Let $E \in \mathcal{E}$, $|E| > 0$, be some generalized edge which connects two inclusions $I_1, I_2 \in \mathcal{I}$. Without loss of generality, let $I_1 = B_{r_1}(0, 0)^T$ and $I_2 = B_{r_2}(0, d)^T$, where $B_r(y)$ denotes the closed disk of radius $r$ around $y$. Let $r_1 \geq r_2$ and $d > r_1 + r_2$. For simplicity, $E$ is supposed to be connected (cf. Remark 3(d) in [8]); otherwise every connected component might be considered on its own.

The subsequent results require a parameterization of the edge $E$. The restriction of $E$ to $I_1, E \cap \partial I_1$, shall be parameterized by some angle $s \in [\alpha, \beta] \subset [-\pi/2, \pi/2]$, i.e., $E \cap \partial I_1 = \phi([\alpha, \beta])$ with $\phi(s) := r_1(s \sin(s), s \cos(s))$. The mapping $\Pi(\cdot, \partial I_2)$
By construction, the product $u$ is parameterized by the diffeomorphism
\[ J : [\alpha, \beta] \times [0, d] \rightarrow \text{int}(E), \quad J(s, \lambda) = (1 - \lambda) \phi(s) + \lambda \Pi(\phi(s), \partial I_2). \] (10)

For any parameter $\eta$, $0 < \eta < \eta_E^{\max} := \min\{[\alpha + \pi/2], [\beta - \pi/2]\}$, a neighborhood of $E$ is defined by $E_\eta := J([\alpha - \eta, \beta + \eta] \times [0, d])$ (see Figure 2.b for an illustration).

**Lemma 3.1.** There exists a constant $C'_E > 0$ which only depends on the ratios $r_2/r_1$, $d/\eta$, and $(\eta_E^{\max} - \eta)^{-1}$ such that for all $u \in H^1_1(E_\eta)$ with $\Delta u \in L^2(E_\eta)$ and $u|_{\partial (I_1 \cup I_2)} = 0$ it holds
\[ \|\nabla^2 u\|_{L^2(E)} \leq C'_E \|\Delta u\|_{L^2(E_\eta)} + \eta^{-1} \|\nabla u\|_{L^2(E_\eta \setminus E)} . \]

**Proof.** We introduce a smooth cut-off function $\psi_{E,\eta} : E_\eta \rightarrow [0, 1]$ with the following properties (see also Remark 3 below):
\[ (\psi_{E,\eta}) = 1, \]
\[ (\psi_{E,\eta})|_{\partial E_\eta \setminus (I_1 \cup I_2)} = 0, \]
\[ \|\nabla^k (\psi_{E,\eta})\|_{L^\infty(E_\eta)} \leq C_{\text{co}} \eta^k \text{ for } k \in \mathbb{N} \cup \{0\}. \] (11)

By construction, the product $u \cdot \psi_{E,\eta}$ vanishes on the boundary of $E_\eta$. Hence, the application of (9) and (11) yields
\[ \|\nabla^2 u\|_{L^2(E)} = \|\nabla^2 (u\psi_{E,\eta})\|_{L^2(E)} \leq \|\nabla^2 (u\psi_{E,\eta})\|_{L^2(E_\eta)} \]
\[ \leq C_{\text{reg}} \|\Delta (u\psi_{E,\eta})\|_{L^2(E_\eta)} \]
\[ \leq C_{\text{co}} C_{\text{reg}} \left( \|\Delta u\|_{L^2(E_\eta)} + 2\eta^{-1}\|\nabla u\|_{L^2(E_\eta \setminus E)} + \eta^{-2}\|u\|_{L^2(E_\eta \setminus E)} \right) . \] (12)

Since $u$ vanishes on $\partial E_\eta \cap (\partial I_1 \cup I_2)$, Friedrichs’ inequality allows one to control the $L^2$ part of the right hand side of (12),
\[ \|u\|_{L^2(E_\eta \setminus E)} \leq d \|\nabla u\|_{L^2(E_\eta \setminus E)}, \]
where $d = \text{dist}(I_1, I_2) + r_1 + r_2$ refers to the distance between the centers of $I_1$ and $I_2$ as above. Thus the assertion is proved with $C'_E = 2C_{\text{co}} C_{\text{reg}} \left( 1 + \frac{2}{\eta} \right)$. \hfill \square
Remark 3. The constant $C_{co}$ in (11) reflects the size of the inclusions $I_1$ and $I_2$ as well as their ratio and, hence, the local uniformity of the distribution of inclusions. It depends on the ratio $r_1/r_2$ and on $(\nu_{\text{max}} - \eta)^{-1}$, where the latter constant becomes large either if the radius $r_1$ tends to zero or if the ratio $\delta_T/\|\delta\|_{L^\infty(\tilde{E})}$ becomes large for some adjacent triangle $T \in \mathcal{T}$. However, the dependence on $\delta_T/\|\delta\|_{L^\infty(\tilde{E})}$ is only an artifact of the way we are cutting $\Omega_{\text{mat}}$ into pieces and could be avoided (e.g., replace $E$ with some suitable sub edge $\tilde{E} \subset E$ and agglomerate the remaining part $E \setminus E$ and the adjacent triangles).

Lemma 3.1 will be applied to certain subdomains of the edge $E$ (subedges) in order to derive estimates in a thickness weighted norm.

Lemma 3.2. If $u \in H^1(E_{\eta})$ with $\Delta u \in L^2(E_{\eta})$ and $u|_{\partial(I_1 \cup I_2)} = 0$, then it holds

(a) $\|\delta \nabla^2 u\|_{L^2(E)} \leq 4C'_E(\|\delta\|_{L^\infty(E_{\eta})}\|\Delta u\|_{L^2(E_{\eta})} + \eta^{-1}\|\nabla u\|_{L^2(E_{\eta})})$

(b) $\|\delta \nabla^2 u\|_{L^2(E)} \leq C'_E(\|\Delta u\|_{L^2(E_{\eta})} + \|\nabla u\|_{L^2(E_{\eta})})$

where $C'_E$ depends only on the constant $C'_E$ from Lemma 3.1.

Proof. We assume $\alpha < \beta = -\alpha$ for simplicity. Let $0 = s_0 < s_1 < s_2 < \ldots < s_J = \beta$ induce a subdivision of $[0, \beta]$. According to $\{s_j\}_{j=1}^J$ we define subsets $E_1, E_2, \ldots, E_{J+1}$ of $E$

$$E_1 := \mathcal{J}([-s_1,s_1]\times[0, d]),$$
$$E_j := \mathcal{J}([-s_j, s_j]\times[0, d]) \setminus E_{j-1} \text{ for } j = 2, 3, \ldots, J, \text{ and}$$
$$E_{J+1} := E_{\eta} \setminus E.$$ 

To prove part (a), the $\{s_j\}_{j=1}^J$ shall be chosen in such a way that

$$\delta_0 := \min_E \delta \quad \text{and}$$
$$\delta_j := \|\delta\|_{L^\infty(E_j)} = \min\{\|\delta\|_{L^\infty(E_j)}, 2\delta_{j-1}\} \text{ for } j = 1, 2, \ldots, J. \quad (14)$$

The application of Lemma 3.1 with $E$ replaced by $\tilde{E}_j := \bigcup_{k=1}^j E_k$, $j = 1, 2, \ldots, J$, yields

$$\|\nabla^2 u\|_{L^2(\tilde{E}_j)} \leq \|\nabla^2 u\|_{L^2(\tilde{E}_j)} \leq C'_E \left(\|\Delta u\|_{L^2(E_{\eta})} + \eta^{-1}\|\nabla u\|_{L^2(E_{\eta})} \right). \quad (15j)$$

The summation of (15j) multiplied by $\delta_j$ over $j = 1$ to $J$ leads to

$$\|\delta \nabla^2 u\|_{L^2(E_{\eta})} \leq \sum_{j=1}^J \|\delta \nabla^2 u\|_{L^2(\tilde{E}_j)} \leq \sum_{j=1}^J \|\nabla^2 u\|_{L^2(E_{\eta})} \quad (15j)$$

$$\leq C'_E \sum_{j=1}^J \delta_j \left(\|\Delta u\|_{L^2(E_{\eta})} + \eta^{-1}\|\nabla u\|_{L^2(E_{\eta})} \right)$$

$$\leq C'_E \left(2\delta_J \|\Delta u\|_{L^2(E_{\eta})} + \eta^{-1}\sum_{j=1}^J \|\nabla u\|_{L^2(E_{\eta})} \sum_{k=1}^{j-1} \delta_k \right) \quad (14)$$

$$\leq 4C'_E \left(\|\delta\|_{L^\infty(E_{\eta})}\|\Delta u\|_{L^2(E_{\eta})} + \eta^{-1}\|\delta \nabla u\|_{L^2(E_{\eta})} \right).$$

To prove the estimate (b) we choose $\{s_j\}_{j=1}^J$ in a different way (yielding a different partition of $E_{\eta}$), i.e.,

$$s_0 := \min_E \delta \quad \text{and}$$
$$s_j := \min\{\beta, 2s_{j-1}\} \text{ for } j = 1, 2, \ldots, J. \quad (16)$$
The actual choice, with regard to the inclusion geometry (convexity of the particles), implies that
\[ s_j \geq \frac{1}{\ell_j} \delta_j := \| \delta \|_{L^\infty(E_j)} \quad \text{for all } j = 1, \ldots, J - 1. \] (17)
The application of Lemma 3.1 with \( E \) replaced by \( E_1 \), and \( E_\eta \) replaced by \( E_1 \cup E_2 \) yields
\[ \| \nabla^2 u \|_{L^2(E_1)} \leq C'_{E, \eta} \left( \| \Delta u \|_{L^2(E_1 \cup E_2)} + s_1^{-1} \| \nabla u \|_{L^2(E_2)} \right). \] (18.1)
The above estimate easily adapts to the case where \( E_1 \) and \( E_2 \) are replaced by some \( E_j \) and \( E_{j+1} \), \( j = 2, 3, \ldots, J \),
\[ \| \nabla^2 u \|_{L^2(E_j)} \leq C'_{E, \eta} \left( \| \Delta u \|_{L^2(E_j \cup E_{j+1} \cup E_{j+2})} + s_j^{-1} \| \nabla u \|_{L^2(E_{j-1} \cup E_{j+1})} \right). \] (18.1)
The summation of (18.1) multiplied by \( \delta_j \) over \( j = 1, \ldots, J \) yields
\[ \| \delta \nabla^2 u \|_{L^2(E)} \leq \sum_{j=1}^{J} \| \delta \nabla^2 u \|_{L^2(E_j)} \leq \sum_{j=1}^{J} \delta_j \| \nabla^2 u \|_{L^2(E_j)} \]
\[ \leq C'_{E, \eta} \sum_{j=1}^{J} \delta_j \left( \| \Delta u \|_{L^2(E_{j-1} \cup E_{j+1})} + s_{j-1}^{-1} \| \nabla u \|_{L^2(E_{j-1} \cup E_{j+1})} \right) \]
\[ \leq (16 + C_s/2) C'_{E, \eta} \left( \| \delta \Delta u \|_{L^2(E_\eta)} + \| \nabla u \|_{L^2(E_\eta)} \right). \]

**Remark 4.** So far, the analysis in this subsection has not considered edges that are related to parts of the outer boundary \( \partial \Omega \). However, by slightly modified arguments, such cases can be treated as well. We have to distinguish two cases.

1. \( E \in \mathcal{E} \) is some generalized edge that connects an inclusion \( I \in \mathcal{I} \) and an artificial inclusion \( H \in \mathcal{H} \) representing a part of the outer boundary \( \partial \Omega \) (see Section 2.2): The previous results apply almost equally, because the boundary part can be regarded as disk with infinite radius.
2. \( E \in \mathcal{E} \) connects two parts of the outer boundary \( H_1, H_2 \in \mathcal{H} \): It might happen that the environment \( E_\eta \) is not contained in \( \Omega_{\text{mat}} \) (see for instance the generalized edges in the corners in Figure 1.b). However, this issue can be cured by simply replacing \( E_\eta \) with \( E_\eta \cap \Omega \) in the upper bounds. Since the solution is given explicitly on \( \partial E_\eta \cap \partial \Omega \), Lemma 3.2 can be generalized in a straightforward way.

In general, the solution of (2) does not vanish on the boundary of the inclusions \( \mathcal{I} \). We, therefore, need to face inhomogeneous boundary data in the regularity estimate. To this end, consider the affine function \( q(s, \lambda) = (1 - \lambda)u_1 + \lambda u_2 \) on the reference edge \( E_{\text{ref}} := [\alpha, \beta] \times [0, d] \) with \( u_k \) being the value of \( u \in V \) at the inclusion \( I_k \), \( k = 1, 2 \). The transformation to \( E \) defines a function
\[ U := q \circ J^{-1}, \] (19)
which is not affine but has a small Hessian \( \nabla^2 U \) in the following sense:
\[ \| \delta \nabla^2 U \|_{L^2(E)} \leq C'_{\gamma} \eta_E^{-1} \| \nabla \eta \|_{L^2(E)}. \] (20)
The constant \( C'_{\gamma} \eta_E^{-1} \) in (20) is related to \( \| J^{-1} \|_{C^2(E_{\text{ref}})} \). Hence, \( C'_{\gamma} \) depends on the ratio \( \eta_E/\eta_{E_{\text{max}}} - \eta_E \), but not on the local thickness \( \delta \).
3.2.2. Interior regularity on triangles. For some \( T \in \mathcal{T} \) and \( \theta \geq 0 \) we denote a scaled version of \( T \) by

\[
T_\theta := \{ x \in T : \text{dist}(x, \partial T) \geq \theta \}.
\]

We employ a cutoff function \( \psi_{T,\theta} \) with

\[
(\psi_{T,\theta})|_{T_\theta} = 1, \quad (\psi_{T,\theta})|_{\partial T} = 0, \quad \text{and}
\]

\[
\|\nabla^k \psi_{T,\theta}\|_{L^\infty(T)} \leq C_\theta^\omega \theta^k \quad \text{for } k \in \mathbb{N} \cup \{0\},
\]

to conclude that for all \( u \in H^1(T) \) with \( \Delta u \in L^2(T) \), it holds that \( u \in H^2(T_\theta) \), and

\[
\|\nabla^2 u\|_{L^2(T_\theta)} \leq \|\nabla^2 (u\psi)\|_{L^2(T)} \leq C_T' \left( \|\Delta u\|_{L^2(T)} + \theta^{-1}\|\nabla u\|_{L^2(T\setminus T_\theta)} + \theta^{-2}\|u\|_{L^2(T\setminus T_\theta)} \right),
\]

where \( C_T' = 2C_\omega^\Delta C_{\text{reg}} \). Note that in fact

\[
\|\nabla^2 u\|_{L^2(T_\theta)} \leq C_T \left( \|\Delta u\|_{L^2(T)} + \theta^{-1}\|\nabla (u - W)\|_{L^2(T\setminus T_\theta)} + \theta^{-2}\|u - W\|_{L^2(T\setminus T_\theta)} \right)
\]

holds with any affine function \( W : T \to \mathbb{R} \), because \( \nabla^2 W \equiv 0 \). Hence, the choice

\[
W = |T|^{-1} \int_T u \, dx \quad \text{together with the Poincaré inequality yields}
\]

\[
\|\nabla^2 u\|_{L^2(T_\theta)} \leq C_T \left( \|\Delta u\|_{L^2(T)} + \theta^{-1}\|\nabla (u - W)\|_{L^2(T)} \right)
\]

with a constant \( C_T \) that depends only on \( C_T' \) and the ratio \( \frac{\theta}{\delta_f} \).

3.3. Global regularity. We simply sum up the local estimates for the elements of \( \mathcal{D} = \mathcal{E} \cup \mathcal{T} \) to derive the global bound. For every edge \( E \in \mathcal{E} \) we choose a parameter \( \eta = \eta_E \) so that

\[
0 < \eta_E < \eta_E^\max \quad \text{and} \quad E_\eta \cap \Omega \subset \text{cl} \left( \Omega_{\text{mat}} \right).
\]

Accordingly, we choose parameters \( \theta = \theta_T > 0 \) for every triangle \( T \in \mathcal{T} \) so that the union of the extended edges and the scaled triangles covers \( \Omega_{\text{mat}} \),

\[
\Omega_{\text{mat}} \subset \bigcup_{E \in \mathcal{E}} E_{\eta/2} \cup \bigcup_{T \in \mathcal{T}} T_\theta.
\]

Some \( \mathcal{D} \)-piecewise constant function \( \sigma : \Omega_{\text{mat}} \to \mathbb{R}_{>0} \) is given by

\[
\sigma|_E = \eta_E \quad \text{for } E \in \mathcal{E} \quad \text{and} \quad \sigma|_T = \theta_T \quad \text{for } T \in \mathcal{T}.
\]

Remark 5. The results of the present section and beyond will depend locally on some negative powers of the parameter function \( \sigma \) defined in (26). Obviously, there exists a constant \( c_T \) such that for all \( K \in \mathcal{D} \), \( \sigma_K \geq c_T \|\delta\|_{L^\infty(K)} \). Since, in this paper, we focus on the dependence of regularity on the thickness function \( \delta \) we do not put any effort in the optimization of our subdivision with regard to the constants \( \sigma \).

For \( u \in V \) we denote its \( T_{\text{mat}} \)-piecewise affine interpolation by \( \mathcal{I}_{\mathcal{D}} u \). More precisely, \( \mathcal{I}_{\mathcal{D}} u \) is defined by (19) on every edge, and \( \mathcal{I}_{\mathcal{D}} u \) is the unique affine interpolant of \( u \) at the vertices of \( T \) on every triangle \( T \in \mathcal{T} \).

**Theorem 3.3.** Let \( u \in V \) be the solution of (3) and \( U_\mathcal{D} := \mathcal{I}_{\mathcal{D}} u \) its \( T_{\text{mat}} \)-piecewise affine interpolation. Then there exists \( C_\mathcal{D} > 0 \), which only depends on the constants of Lemma 3.2 and (23.b), such that

\[
\|\delta \nabla^2 u\|_{L^2(\Omega_{\text{mat}})} \leq C_\mathcal{D} \left( \|\delta f\|_{L^2(\Omega_{\text{mat}})} + \|\sigma^{-1}\delta \nabla U_\mathcal{D}\|_{L^2(\Omega_{\text{mat}})} \right).
\]
Proof. We decompose \( u = (u - u_{\text{har}}) + (u_{\text{har}} - U_{\text{har}}) + (U_{\text{har}} - U_D) + U_D, \) where \( u_{\text{har}} \in H^1(\Omega_{\text{mat}}) \) denotes the unique harmonic function with trace \( u|_{\partial \Omega_{\text{mat}}} \), and \( U_{\text{har}} \) the \( D \)-piecewise harmonic function which equals \( U_D \) on the boundary of every element \( K \in D \). The application of the triangle inequality yields
\[
\|\Delta \nabla u\|_{L^2(\Omega_{\text{mat}})} \leq \|\Delta \nabla (u - u_{\text{har}})\|_{L^2(\Omega_{\text{mat}})} + \|\Delta \nabla (u_{\text{har}} - U_{\text{har}})\|_{L^2(\Omega_{\text{mat}})} + \|\Delta \nabla (U_{\text{har}} - U_D)\|_{L^2(\Omega_{\text{mat}})} + \|\Delta \nabla U_D\|_{L^2(\Omega_{\text{mat}})}
\]
where the constant \( C \) depends only on the constants of Lemma A.1.

The estimate
\[
M_1^{(25)} \leq \sum_{T \in T} \|\Delta \nabla (u - u_{\text{har}})\|_{L^2(\Omega_{\text{mat}})}^2 + \sum_{E \in E} \|\Delta \nabla (u - u_{\text{har}})\|_{L^2(E_{\eta/2})}^2
\]
holds with a constant \( C_1 \) which depends only on the constants of Lemma 3.2.a and (23). Since \( (u - u_{\text{har}}) \in H^1_0(\Omega_{\text{mat}}) \), we have from (3.a) and a localized version of the Friedrichs' inequality (see Lemma A.1),
\[
\|\nabla (u - u_{\text{har}})\|_{L^2(\Omega_{\text{mat}})} \leq C_F \|\nabla f\|_{L^2(\Omega_{\text{mat}})}.
\]

Since \( u_{\text{har}} - U_{\text{har}} \) is locally harmonic, the application of Lemma 3.2.a locally on \( E_{\eta/2}, E \in E \) and (23) on \( T_\Theta, T \in T \), yields
\[
M_2 \leq C_2 \|\sigma^{-1} \nabla (u_{\text{har}} - U_{\text{har}})\|_{L^2(\Omega_{\text{mat}})}
\]
where the constant \( C_2 \) depends only on \( C_E \) and \( C_T \). From Lemma A.2, we also get
\[
M_2 \leq C_2 \|\sigma^{-1} \nabla U_D\|_{L^2(\Omega_{\text{mat}})}.
\]

Finally, the application of Lemma 3.2.b on every \( E \in E \), yields
\[
M_3 \leq C_3 \|\Delta U_D\|_{L^2(\Omega_{\text{mat}})}^2 + \sum_{E \in E} \|U_{\text{har}} - U_D\|_{L^2(E)}^2
\]
where the constant \( C_3 \) depends only on \( C''_E \). The definition of \( U_{\text{har}} \), (20), and Lemma A.1 yield
\[
M_3 \leq C_3 \|\sigma^{-1} \nabla U_D\|_{L^2(\Omega_{\text{mat}})}.
\]

The assertion follows readily by combining (27), (28), (29), and (30).

\[\square\]

**Lemma 3.4.** Let \( u \in V \) be the solution of (3) and \( U_D := \mathcal{I}_D u \) its \( T_{\text{mat}} \)-piecewise affine interpolation. Then it holds
\[
\|\Delta \nabla U_D\|_{L^2(\Omega_{\text{mat}})} \leq C_3 \left( \|f\|_{L^2(\Omega_{\text{mat}})} + \|U_D\|_{L^\infty(\partial \Omega_{\text{mat}})} \right)
\]
with some constant \( C_3 \) that does not depend on \( \delta \).

**Proof.** By an inverse inequality we get
\[
\|\Delta \nabla U_D\|_{L^2(\Omega_{\text{mat}})} \leq \|U_D\|_{L^2(\Omega_{\text{mat}})}.
\]
Moreover,
\[ \| U_D \|_{L^2(\Omega^{\text{mat}})} \leq C_f' \| u \|_{L^2(\Omega^{\text{mat}})} \leq C_f' \left( \| u - u^{\text{har}} \|_{L^2(\Omega^{\text{mat}})} + \| u^{\text{har}} \|_{L^2(\Omega^{\text{mat}})} \right), \]
where we have used the boundedness of the interpolation operator \( \mathcal{I}_D \), the maximum principle for second order elliptic operators (see [6, Theorem 6.4.1]) and a classical \( L^2 \) a priori estimate (see [6, Theorem 6.2.6]).

**Theorem 3.5.** Let \( u \in V \) be the solution for (3). Then there exists \( C_{u_D,f,\sigma} > 0 \), which depends only on the data \( f \) and \( u_D \), on \( \sigma \) defined in (26), and the constants of Theorem 3.3 and Lemma 3.4, such that
\[ \| \delta \nabla^2 u \|_{L^2(\Omega^{\text{mat}})} \leq C_{u_D,f,\sigma}. \]

**Proof.** The proof follows readily by combining Theorem 3.3 and Lemma 3.4. \( \square \)

4. **Stable approximation close to percolation.** We now consider any appropriate conforming finite element approximation of (3). Let \( V_h \subset V \) be some finite dimensional subspace of \( V \). The corresponding discrete variational problem reads: Find \( u_h \in V_h \) such that
\[ \int_{\Omega^{\text{mat}}} \nabla u_h(x) \nabla v_h(x) \, dx = \int_{\Omega^{\text{mat}}} f(x) v_h(x) \, dx \quad \text{for all} \quad v_h \in V_h \cap H^1_0(\Omega^{\text{mat}}), \quad (31.a) \]
\[ u_h = u_D \quad \text{on} \quad \partial \Omega. \quad (31.b) \]

It is assumed for simplicity that the Dirichlet data \( u_D \) is resolved by \( V_h \), i.e., there is some \( v_h \in V_h \) such that \( v_h|_{\partial \Omega} = u_D \). The discrete space \( V_h \) shall consist of functions that are piecewise smooth with respect to some mesh \( \mathcal{G} \) of \( \Omega^{\text{mat}} \). The mesh \( \mathcal{G} \), which consist of possibly curved elements, is supposed be conforming in the sense that \( \cup \mathcal{G} = \bar{\Omega} \). Its mesh width is denoted by \( h : \Omega^{\text{mat}} \to \mathbb{R}_{>0}, h|_K := h_K := \text{diam}(K) \) for all \( K \in \mathcal{G} \). Clearly, there holds \( h \leq C_0 \delta \) with some constant \( C_0 \) which is related to shape regularity of the elements, i.e., the ratio between the radius of the largest ball that can be inscribed in an element and the radius of the smallest ball that contains the element. We assume that the space \( V_h \) satisfies approximation properties locally, i.e., there exists some constant \( C_{\text{appr}} \) so that for all \( K \in \mathcal{G} \) and all \( u \in H^2(K) \),
\[ \inf_{v_h \in V_h} (h_K^{-1} \| u - v_h \|_{L^2(K)} + \| \nabla (u - v_h) \|_{L^2(K)}) \leq C_{\text{appr}} h_K \| \nabla^2 u \|_{L^2(K)}. \quad (32) \]

**Theorem 4.1.** If \( u \in V \) is the solution for (3), and \( u_h \in V_h \) its Galerkin approximation that solves (31), then
\[ \| \nabla (u - u_h) \|_{L^2(\Omega^{\text{mat}})} \leq C_{f,u_D,V_h} \| h/\delta \|_{L^\infty(\Omega^{\text{mat}})} \]
holds with \( C_{f,u_D,V_h} = C_{\text{appr}} C_{u_D,f,\sigma} \) where \( C_{\text{appr}} \) is the constant from (32) and \( C_{u_D,f,\sigma} \) the one from Theorem 3.5.

**Proof.** The optimality of the Galerkin method in energy norm together with the approximation properties of the space \( V_h \) (cf. (32)) imply that
\[ \| \nabla (u - u_h) \|_{L^2(\Omega^{\text{mat}})} \leq C_{\text{appr}} \| h \nabla^2 u \|_{L^2(\Omega^{\text{mat}})}. \quad (33) \]

Using the assumption that the ratio \( h/\delta \) is bounded and applying Theorem 3.5 we further estimate
\[ \| h \nabla^2 u \|_{L^2(\Omega^{\text{mat}})} \leq \| h/\delta \|_{L^\infty(\Omega^{\text{mat}})} \| \delta \nabla^2 u \|_{L^2(\Omega^{\text{mat}})} \leq C_{u_D,f,\sigma} \| h/\delta \|_{L^\infty(\Omega^{\text{mat}})}. \quad (34) \]

The combination of (33) and (34) yields the assertion. \( \square \)
In practical computations, the assumption of conformity $\cup \mathcal{G} = \overline{\Omega}$ might be relaxed. E.g., the inclusions might by approximated by linear, quadratic, or cubic splines. The resulting geometries are supported by many state-of-the-art mesh generators. However, such a perturbation of the original geometry can only lead to a meaningful approximation if it preserves the distance between neighboring inclusions very precisely.

A special choice of the mesh $\mathcal{G}$ and the corresponding space $V_h$ which preserves conformity is discussed in [10] where

$$\mathcal{G} = \mathcal{D} \text{ and } V_h = V_\mathcal{D} := \{ v \in C^0(\Omega^{\text{mat}}) : v \text{ is } T_{\text{mat}}\text{-piecewise affine}\}.$$  

**Corollary 4.2.** If $u \in V$ is the solution for (3) and $u_h \in V_\mathcal{D}$ its Galerkin approximation that solves (31), then

$$\|\nabla (u - u_h)\|_{L^2(\Omega^{\text{mat}})} \leq C_{I_p,\mathcal{D}} C_{u,\mathcal{D},f,\sigma},$$

where the constant $C_{I_p,\mathcal{D}}$ is related to the approximation property of $V_\mathcal{D}$ (see [10, Theorem 3.1, Corollary 3.3]).

**Proof.** The proof follows readily by combining Theorem 4.1 and the approximation property of the space $V_\mathcal{D}$ provided by [10, Theorem 3.1, Corollary 3.3].

5. **Conclusion.** In this paper, we have proved that conforming finite element methods yield approximations of the temperature distribution in particle reinforced composite materials that are robust with respect to critical geometric parameters of the packing of particles. More precisely, the absolute error of such an approximation can be bounded by some universal constant that does not depend on the geometry of the particle distribution. The relative error scales inversely proportional to the energy of the material. Conforming finite element methods allow one to trace a possible blow-up of the energy as the thickness tends to zero on a path of inclusions that separates the domain. Hence, material simulations based on those methods are able to capture the phase transition from low conductivity to high conductivity (percolation) as the volume fraction of particles is increased.

Moreover, given a fixed sample of the geometry of the material, the regularity theory presented here shows that the use of a conforming finite element mesh with local width proportional to the local thickness of the matrix material guarantees accurate results. Therefore, finite element methods might be used to compute effective properties of a specific sample of the material. These effective properties can then be used as the basis of an numerical upscaling procedure which simulates global material behavior.

The theory presented in this paper can be extended to the case of general smooth inclusions. The same holds true for 3-dimensional setting and for the consideration of general second order elliptic differential operators.

**Appendix A. Inequalities.** We now prove a version of Friedrichs’ inequality that is local with respect to the thickness of the domain.

**Lemma A.1.** There is some constant $C_F$ which does not depend on $\delta$ such that for all $v \in H^1_0(\Omega^{\text{mat}})$, it holds that

$$\|v\|_{L^2(\Omega^{\text{mat}})} \leq C_F \|\delta \nabla v\|_{L^2(\Omega^{\text{mat}})}.$$
For any $\varepsilon > 0$, Young’s inequality yields

$$\|\delta \|_{L^\infty(\Omega)} \leq \frac{1}{2} \|\nabla (u - v)\|_{L^2(\Omega)}.$$
Choosing $\varepsilon = (2C)^{-2}$ proves the assertion.

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