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THE PENETRATION FUNCTION AND ITS APPLICATION TO MICROSCALE PROBLEMS*

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Abstract.

The penetration function measures the effect of the boundary data on the energy of the solution of a second order linear elliptic PDE taken over an interior subdomain. Here the coefficients of the PDE are functions of position and often represent the material properties of non homogeneous media with microstructure. The penetration function is used to assess the accuracy of global-local approaches for recovering local solution features from coarse grained solutions such as those delivered by homogenization theory.

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1 Introduction.

Let us consider the elliptic problem on a bounded domain $\Omega \subset R^2$ with piecewise smooth Lipschitz boundary Γ

$$\operatorname{div} \mathbf{A}(x) \operatorname{grad} u(x) = f \quad \text{on } \Omega, \tag{1.1a}$$

$$u(x) = g(x) \quad \text{on } \partial\Omega = \Gamma, \tag{1.1b}$$

or

$$\partial u(x)/\partial n_c = h(x) \quad \text{on } \partial\Omega = \Gamma, \tag{1.1c}$$

where

$$\mathbf{A}(x) = \{a_{i,j}(x),\ a_{i,j}(x) \in L^\infty(\Omega),\ i,j = 1,2\}$$

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is a symmetric positive matrix satisfying the coercivity condition

$$\gamma_1|\xi|^2 \leq \xi^T \mathbf{A}(x)\xi \leq \gamma_2|\xi|^2, \quad 0 < \gamma_1 < \gamma_2 < \infty. \tag{1.2}$$

In general we assume that $a_{i,j}(x) \in L^\infty(\Omega)$ are only measurable functions, but we will also consider other classes Υ *of* $\mathbf{A}$. For example we will consider the class Υ_0 of isotropic matrices for which $a_{1,2} = a_{2,1} = 0$, $a_{1,1}(x) = a_{2,2}(x)$ and

$$a_{1,1}(x) = \gamma_1 \quad \text{or} \quad a_{1,1}(x) = \gamma_2,$$

i.e., $a_{1,1}(x)$ takes only one of two values γ_1 or γ_2 depending on x.

We introduce the bilinear form $B(u,v)$ defined on $\mathrm{H}^1(\Omega) \times \mathrm{H}^1(\Omega)$ given by

$$B(u,v) = \int_\Omega (\nabla v)^T \mathbf{A}(x)(\nabla u)dx \tag{1.3}$$

and

$$F \in (\mathrm{H}^1(\Omega))^*. \tag{1.4}$$

If $g = G/\Gamma \in \mathrm{H}^{1/2}(\Gamma)$, $G \in \mathrm{H}^1(\Omega)$ and $f \in \mathrm{L}_2(\Omega)$, then the solution u of (1.1) satisfies

$$u = G + u_0, \quad u_0 \in \mathrm{H}_0^1(\Omega) \tag{1.5}$$

and for all $v \in \mathrm{C}_0^\infty(\Omega)$

$$B(u_0 + G, v) = F(v) = \int_\Omega fvdx. \tag{1.6}$$

The solution exists and is unique. If $h \in \mathrm{H}^{-1/2}(\Gamma)$ and $\int_\Gamma hds + \int_\Omega fdx = 0$, then the solution $u \in \mathrm{H}^1(\Omega)$ of (1.1) satisfies

$$B(u,v) = F(v) = \int_\Gamma hvds + \int_\Omega fvdx \tag{1.7}$$

for all $v \in \mathrm{C}^\infty(\Omega)$. It exists and is unique up to an additive constant. We denote the energy norm by $\|u\|_{E(\Omega)} = (B(u,u))^{1/2}$ and the associated energy space by E. The energy norm is equivalent to the $\mathrm{H}^1(\Omega)$ norm. If $\mathbf{A}$ is only measurable then the solution u is in the space $H^1(\Omega)$, however if $\mathbf{A}$ is constant and $f = 0$ then the solution u is analytic in Ω (but not in $\overline{\Omega}$). Here it is noted that the assumption $\Omega \subset R^2$ is not necessary and is made to illustrate the ideas.

The numerical treatment of the problem (1.1) is usually directly or indirectly related to a homogenization approach. The theory of homogenization in its most general formulation is described by the theory of G-convergence [30], or the H-convergence theory when nonsymmetric matrices are considered [25]. Here we consider a sequence of matrices $\mathbf{A}_n(x)$, $n = 1, 2, \ldots$, which converges in the sense of the G-convergence to the limit $\mathbf{A}_H(x)$. In this context the homogenized solution u_H satisfies (1.1) when $\mathbf{A}$ is replaced by $\mathbf{A}_H$. The solution u_n of the problem (1.1) with $\mathbf{A} = \mathbf{A}_n$ converges to u_H in $\mathrm{L}_2(\Omega)$ but not in $H^1(\Omega)$. However the energies $\int_\Omega (\nabla u_n)^T \mathbf{A}_n (\nabla u_n) dx$ converge to $\int_\Omega (\nabla u_H)^T \mathbf{A}_H (\nabla u_H) dx$ see, [30, 25]. The reader is referred to [30] and [25] for a full accounting of the theory of G (or H) convergence, see also [15].

For the periodic matrices $\mathbf{A}_\epsilon(x) = \mathbf{A}(x/\epsilon)$, $\epsilon > 0$, $\epsilon \to 0$ the homogenization theory is well developed, see e.g. [6]. Here explicit formulas for $\mathbf{A}^H$ are available. Nevertheless there are still open questions related to the decay of boundary layers and the behavior of the solution in the neighborhood of singular points and near corner points on the boundary. The exposition presented in [2] among others provides a history of numerical approaches for replacing the microscale equation by the macroscale solution. There are many different computational approaches for solving problems with microscale, see e.g., [1, 3, 10, 11, 14, 31, 32]. Methods suitable for problems arising in the context of composite materials are introduced in [4, 8] see also [9].

This paper examines the problem of how to accurately recover the microscale features of the solution of (1.1) from the known macroscopic (homogenized) solution. An approach to this problem is suggested for example in [1, Section 3.5] or [27]. The main idea behind the recovery of the microscale information inside a subdomain $\omega \subset \Omega$ is the classical, widely used, idea of the global-local approach. In this context if the crude (homogenized) solution U_H is known then on ω the actual solution u is approximated by the solution u_ω of (1.1a) with the boundary condition

$$u_\omega(x) = U_H(x) \quad \text{on } \partial\omega$$

or

$$\partial u_\omega / \partial n_c = \partial U_H / \partial n_c \quad \text{on } \partial\omega,$$

where $\partial u_\omega / \partial n_c$ is the conormal derivative with respect to $\mathbf{A}(x)$ and $\partial U / \partial n_c$ is the conormal derivative with respect to $\mathbf{A}_H(x)$. One then considers the accuracy of the approximation u_ω on subdomains $\tilde{\omega} \subset \omega$. It is tacitly assumed that the error $\|u - u_\omega\|_{E(\widetilde{\omega})}$ is small provided that $\partial\widetilde{\omega}$ is not close to $\partial\omega$. We will show that this assumption is in general false. We will develop lower and upper bounds for $\|u - u_\omega\|_{E(\widetilde{\omega})}$ when the homogenized solution U_H is known.

The homogenized solution U_H is usually smooth (possibly analytic) and on $\partial\omega$ it can be well approximated by an m-dimensional space, so that only m coefficients are available for disposition. If U_H is analytic then m is very small since U_H is well approximated by polynomials of low degree.

For a selected m dimensional space V_m, respectively for a sequence of spaces $\{V_m\}$, we are interested in

$$\inf_{\chi \in V_m} \|u - \chi\|_{E(\widetilde{\omega})}$$

where u is the solution of (1.1) about which we know only that $u \in \mathrm{H}^1(\omega)$ and $u \in \mathrm{H}^{1/2}(\partial\omega)$.

We will show that in the general case we have the lower bound

$$\inf_{\chi \in V_m} \|u - \chi\|_{E(\widetilde{\omega})} \geq C m^{-1/2+\epsilon}$$

and for the upper bound

$$\inf_{\chi \in V_m} \|u - \chi\|_{E(\widetilde{\omega})} \leq C m^{-\delta}$$

where $\delta > 0$ depends on γ_1, γ_2 in (1.2). The maximal (or sup) δ is not known.

Let us assume that the numerical homogenized solution was obtained by the finite element method with size Δ. Then in general these results show that we cannot retrieve the microscopic features of the solution with an accuracy better than $\mathrm{O}(|\partial\omega|/\Delta)^{-1/2}$ where $|\partial\omega|$ is the length of the boundary $\partial\omega$. We will see later that the retrieval could be worse depending for example on the contrast γ_2/γ_1 in (1.2), see Section 5.2.

The aforementioned bounds apply to the general class of matrices $\mathbf{A}$. It remains to be seen what new estimates hold for different classes Υ of $\mathbf{A}$.

2 The penetration function.

Let $\omega \subset \Omega$, $d = \mathrm{dist}(\omega, \partial\Omega)$ and $\mathbf{V}_n \subset \mathrm{H}^{1/2}(\partial\Omega)$, $n = 1, 2, \ldots$ be $m(n)$ dimensional spaces. Let

$$\mathrm{W}_n = \big\{ v \in \mathrm{H}^1(\Omega) \mid v \text{ satisfies (1.1) with } f = 0 \text{ and } v/\partial\Omega \in \mathbf{V}_n \big\}. \tag{2.1}$$

Further let $g \in \mathrm{H}^{1/2}(\partial\Omega)$ and $u(g) \in E$ be the solution of (1.1a), (1.1b) with $f = 0$. We define the penetration function $\Xi(\mathbf{V}_n, d)$:

$$\Xi(\mathbf{V}_n, d) = \Xi(n, d) = \sup_{\|g\|_{\mathrm{H}^{1/2}(\partial\Omega)} = 1} \big\{ \inf_{w \in \mathrm{W}_n} \|u(g) - w\|_{E(\omega)} \big\}. \tag{2.2}$$

The penetration function $\Xi(n, d)$ depends on the sequence $\{\mathbf{V}_n\}$, $n = 1, 2, \ldots$ and on the class Υ of matrices $\mathbf{A}$ under consideration. If $m(n) = n$ then we will be interested in the estimate of $\Xi(n, d)$ of the form $\Xi(n, d) \leq C n^{-\beta}$. We will be interested in the maximal β in the sense that $\limsup_{n\to\infty} \Xi(n, d) n^{\beta} < \infty$. Obviously the penetration function $\Xi(n, d)$ is a measure of our ability to retrieve the details of the micro solution with a desired accuracy.

The penetration function respectively the error of the retrieval depends on $\{\mathbf{V}_n\}$. Hence the question arises what is the optimal selection of the spaces $\mathbf{V}_n$. This question is naturally related to the Kolmogorov n-width [29] and we define

$$\Theta(m(n), d) = \inf_{\mathbf{V}_n} \Xi(\mathbf{V}_n, d), \quad \dim \mathbf{V}_n = m(n).$$

In this discussion we have assumed that $f = 0$ and in the applications this is often the case. However if $f \neq 0$ then we can eliminate f by a particular solution and the previous considerations hold. So far we have defined the penetration function for the Dirichlet boundary condition (1.1b). The penetration function for the Neumann boundary condition (1.1c) is completely analogous.

3 Weighted Sobolev spaces and the penetration function.

For points x inside Ω we let $\mathrm{d}(x)$ denote the distance of x to the boundary $\partial\Omega$. Then for $|\alpha| < 1$ we define

$$\mathrm{H}^{1,\alpha}(\Omega) = \left\{ u \,\Big|\, \int_\Omega |\nabla u|^2 \mathrm{d}^\alpha dx = \|u\|_{1,\alpha}^2 < \infty \right\}$$

and take $\mathrm{H}_0^{1,\alpha}(\Omega)$ to be the closure of the space $\mathrm{C}_0^\infty(\Omega)$ in the norm $\| \, \|_{1,\alpha}$.

REMARK 3.1. For $\alpha > 1$ the space $\mathrm{H}_0^{1,\alpha}(\Omega)$ is dense in $\mathrm{H}^1(\Omega)$.

REMARK 3.2. In this treatment we will consider the spaces $\mathrm{H}_0^{1,\alpha}(\Omega)$ and $\mathrm{H}_0^{1,-\alpha}(\Omega)$ for $|\alpha| < 1$.

Let us now define the Dirichlet problem over the weighted Sobolev spaces. The bilinear form (1.3) is well defined on $H_0^{1,\alpha}(\Omega) \times H_0^{1,-\alpha}(\Omega)$ and is continuous.

Let $0 \le \alpha < 1$, $G \in \mathrm{H}^1(\Omega)$, $g = G/\partial\Omega \in \mathrm{H}^{1/2}(\partial\Omega)$ and $F \in (\mathrm{H}_0^{1,-\alpha}(\Omega))^*$, then $u \in \mathrm{H}^{1,\alpha}(\Omega)$ is the solution of the Dirichlet problem if

a. $u = G + u_0$, $u_0 \in \mathrm{H}^{1,\alpha}(\Omega)$,
b. $B(G + u_0, v) = F(v)$, for any $v \in \mathrm{H}_0^{1,-\alpha}(\Omega)$.

We have

THEOREM 3.1 ([26]). *Suppose the bilinear form $B(u,v)$ is defined and continuous on $H_0^{1,\alpha}(\Omega) \times H_0^{1,-\alpha}(\Omega)$ with $0 \le \alpha < 1$ and*

$$\inf_u \sup_v |B(u,v)| \ge c_1 > 0, \quad \|u\|_{1,\alpha} = 1, \quad \|v\|_{1,-\alpha} = 1, \tag{3.1a}$$

$$\inf_v \sup_u |B(u,v)| \ge c_2 > 0, \quad \|u\|_{1,\alpha} = 1, \quad \|v\|_{1,-\alpha} = 1, \tag{3.1b}$$

$$F \in \left(\mathrm{H}_0^{1,-\alpha}(\Omega)\right)^*, \tag{3.1c}$$

then there exists a unique solution $u \in \mathrm{H}_0^{1,\alpha}(\Omega)$ such that

$$B(u,v) = F(v) \quad \textit{for any } v \in \mathrm{H}_0^{1,-\alpha}(\Omega) \tag{3.2a}$$

and

$$\|u\|_{1,\alpha} \le C\|F\|_{1,-\alpha}^*, \quad \|F\|_{1,\alpha}^* = \sup v \frac{|F(v)|}{\|v\|_{1,-\alpha}}. \tag{3.2b}$$

The following Theorem 3.2 follows from the embedding theorems for weighted Sobolev spaces (see [16]).

THEOREM 3.2. *There exists $\delta > 0$ such that for any $0 < \alpha < \delta$ the conditions* (3.1a), (3.1b) *hold and hence the solution $u \in \mathrm{H}^{1,\alpha}$ of the Dirichlet problem exists and* (3.2b) *holds.*

The major problem is to determine the value δ. This value can be determined from the analysis of the embedding theorems for Sobolev weighted spaces. For example by an easy analysis we could obtain an estimate $\delta = \lambda/(2+\lambda)$ where $\lambda = \gamma_1/\gamma_2$ but this value is pessimistic. Also from [7, 22] an estimate for δ can be obtained. Once more it will be pessimistic. We are of course interested in $\sup\delta$. Note that for $\alpha = 0$ the conditions (3.1a), (3.1b)) are trivially satisfied.

We now apply Theorems 3.1 and 3.2 to obtain an upper estimate for the penetration function $\Xi(\mathbf{V}_n, d)$. First we introduce some useful notation. If $g \in \mathrm{H}^{1/2}(\partial\Omega)$, we denote by $\psi(g) \in \mathrm{H}^1(\Omega)$ the solution of (1.1a), (1.1b) with $f = 0$ and $\mathbf{A} = \mathbf{I}$.

We prove now the following Theorem 3.3:

THEOREM 3.3. *Let* $0 \le \alpha < \delta$ *as in the Theorem 3.2. Further let* $\mathbf{V}_n \subset \mathrm{H}^{1/2}(\partial\Omega)$ *be* $m(n)$ *dimensional space and assume that for any* $v \in \mathrm{H}_0^{1,-\alpha}(\Omega)$,

$$\inf_{z\in\mathbf{V}_n} |B((\psi(g)-\psi(z)),v)| \le S(g,\mathbf{V}_n)\|v\|_{1,-\alpha} \tag{3.3}$$

$$S(g,\mathbf{V}_n) \le Q(\mathbf{V}_n)\|g\|_{\mathrm{H}^{1/2}(\partial\Omega)}, \tag{3.4}$$

then

$$\Xi(n,d) \le CQ(\mathbf{V}_n)d^{-\alpha/2}. \tag{3.5}$$

PROOF. Let $u(g)$ respectively $w(z)$ be the solution of (1.1a) with $u(g) = g$ respectively $w(z) = z \in \mathbf{V}_n$ on $\partial\Omega$. Then $u(g) - w(z) = \psi(g) - \psi(z) + u_0$ and because we assumed that $f = 0$ the function $u_0 \in \mathrm{H}_0^1(\Omega)$ satisfies for all $v \in \mathrm{H}_0^{1,-\alpha}(\Omega) \subset \mathrm{H}_0^1(\Omega)$ the equation $B(u_0, v) = -B(\psi(g)-\psi(z), v)$. From this we get

$$\|u_0\|_{1,\alpha} \le S(g,\mathbf{V}_n).$$

Because Theorem 3.2 holds also for $\mathbf{A} = \mathbf{I}$, we get

$$\|\psi(g)-\psi(z)\|_{1,\alpha} \le CS(g,\mathbf{V}_n)$$

and (3.5) follows immediately from (3.4). □

Let us consider now a special case when Ω is the unit disk

$$\Omega = \{r, \Theta \mid 0 \le r < 1,\ 0 \le \Theta < 2\pi\}.$$

Note that any $g \in \mathrm{H}^{1/2}(\partial\Omega)$ can be written in the form

$$g(\Theta) = \sum_{k=0}^{\infty} a_k \cos k\Theta + \sum_{k=1}^{\infty} b_k \sin k\Theta$$

and

$$\|g\|^2_{\mathrm{H}^{1/2}(\partial\Omega)} = \pi\Big(2a_0^2 + \sum_{k=1}^{\infty}\big(a_k^2 + b_k^2\big)\Big).$$

Further

$$\psi(g) = \sum_{k=0}^{n} a_k r^k \cos k\Theta + \sum_{k=1}^{n} b_k r^k \sin k\Theta. \tag{3.6}$$

Based on this we select

$$\mathbf{V}_n = \left\{ z(\Theta) \,\middle|\, z(\Theta) = \sum_{k=0}^{n} c_k \cos k\Theta + \sum_{k=1}^{n} d_k \sin k\Theta,\ c_k,\ d_k \in \mathbf{R} \right\} \tag{3.7}$$

and $\mathbf{V}_n$ has dimension $m = 2n + 1$. For

$$z(\Theta) = \sum_{k=n+1}^{\infty} a_k \cos k\Theta + \sum_{k=n+1}^{\infty} b_k \sin k\Theta$$

we get

$$\psi(g) - \psi(z) = \sum_{k=n+1}^{\infty} a_k r^k \cos k\Theta + \sum_{k=n+1}^{\infty} b_k r^k \sin k\Theta.$$

By an easy computation we get

$$S(g, \mathbf{V}_n) \le C n^{-\alpha/2} \log^{\alpha/2} n \|g\|_{\mathrm{H}^{1/2}(\partial\Omega)}. \tag{3.8}$$

Hence from the Theorem 3.3 we get

THEOREM 3.4. *Let $\Omega \subset \mathbf{R}^2$ be the unit disk and $\mathbf{V}_n \in \mathrm{H}^{1/2}(\partial\Omega)$ be the space of trigonometric polynomials of degree n on $\partial\Omega$. If $\mathbf{A}$ satisfies condition* (1.2) *then there exists $0 < \alpha < 1$ such that*

$$\Xi(\mathbf{V}_n, d) < C(d) n^{-\alpha/2} \log^{\alpha/2} n. \tag{3.9}$$

REMARK 3.3. The inequality (3.9) delivers an upper bound for the penetration function that depends on the value α respectively δ. Later in Section 5.2 we will see by a numerical investigation that this estimate is very pessimistic for the class Υ_0 of $\mathbf{A}$.

If $\mathbf{A} = \mathbf{I}$ we use (3.6) to immediately deduce the following theorem.

THEOREM 3.5. *Let $\mathbf{A} = \mathbf{I}$, Ω is the unit disk and $\mathbf{V}_n$ is the space of trigonometric polynomials of degree n on $\partial\Omega$. Then*

$$\Xi(\mathbf{V}_n, d) < C e^{-n} \tag{3.10}$$

REMARK 3.4. The estimate (3.10) holds for the entire class Υ of matrices $\mathbf{A}$ which are analytic on $\overline{\Omega}$.

REMARK 3.5. Theorem 3.5 is related to the well known Saint Venant principle and Theorem 3.4 can be understood as a generalization of the Saint Venant principle.

When Ω is the unit disk we selected a special space $\mathbf{V}_n$, namely the space of trigonometric polynomials on $\partial\Omega$ for which (3.3) and (3.4) hold. For generic domains Ω the spaces $\mathbf{V}_n$ have to be selected so that (3.3) and (3.4) are satisfied. These choices of $\mathbf{V}_n$ are also naturally related to the Kolmogorov n-width functions on $\partial\Omega$ see, [29].

We conclude noting that we have obtained upper bounds on the penetration function for Dirichlet boundary conditions. The results obtained for the Dirichlet case apply to Neumann boundary conditions as well since we can appeal to the dual formulation which transforms the Neumann boundary conditions into Dirichlet boundary conditions.

4 The lower estimate for the penetration function.

In Section 3 we considered the case when the domain Ω was the unit disk. This is equivalent with the problem which is periodic in a strip.

Let

(4.1)

$$\Omega = \{x = (x_1, x_2) \mid x_1 \in \Gamma = (-\pi, \pi],\ 0 \le x_2 \le q < \infty\}$$

$$\Omega_l = \{x \mid x_1 \in \Gamma,\ l < x_2 < q\} \quad \text{and}$$

$$\mathbf{H} = \big\{u \in \mathrm{H}^1(\Omega) | \, u \text{ is } 2\pi \text{ periodic in } x_1 \text{ and symmetric with respect to } x_1 = 0\big\}.$$

We consider now the differential equation (1.1a) on Ω with $\mathbf{A}$ satisfying (1.2) and $\mathbf{A}(x_1, x_2) = \mathbf{A}(-x_1, x_2)$ with $f = 0$ and boundary conditions

$$u(-\pi, x_2) = u(\pi, x_2) \tag{4.2a}$$

$$\partial u(x)/\partial n_c = h(x_1) \in \mathrm{H}^{-1/2}(\Gamma), \quad x_1 \in \Gamma,\ x_2 = 0 \tag{4.2b}$$

$$\partial u(x)/\partial n_c = 0 \quad \text{on } x_1 \in \Gamma,\ x_2 = q \tag{4.2c}$$

where $u(x_1, x_2)$, $h(x_1)$ are symmetric with respect to $x_1 = 0$, 2π-periodic and $\int_\Gamma h(x_1) dx_1 = 0$. The solution $u \in \mathrm{H}^1(\Omega)$ of the Neumann problem stated above exists and is unique up to a constant function.

Any $h(x_1) \in \mathrm{H}^{-1/2}(\Gamma)$, symmetric and 2π-periodic can be written in the form

$$h(x_1) = \sum_{k=1}^{\infty} a_k \cos kx_1 \tag{4.3}$$

with

$$\|h\|^2_{\mathrm{H}^{-1/2}(\Gamma)} = \sum_{k=1}^{\infty} a_k^2 k^{-1} < \infty. \tag{4.4}$$

For h_1, $h_2 \in \mathrm{H}^{-1/2}(\Gamma)$, $h_1(x_1) = \sum_{k=1}^{\infty} a_k \cos kx_1$, $h_2(x_1) = \sum_{k=1}^{\infty} b_k \cos kx_1$ we can define a scalar product

$$\langle h_1, h_2 \rangle = \sum_{k=1}^{\infty} a_k b_k k^{-1}.$$

The Neumann problem creates the mapping of $\mathrm{H}^{-1/2}(\Gamma)$ into $\mathbf{H}$ given in (4.1). As before we denote $u(h)$ the solution of the Neumann problem satisfying the conditions (4.2).

Let

$$\mathcal{S}_n(\Gamma) = \Big\{ v \in \mathrm{H}^{-1/2}(\Gamma) \,\Big|\, v = \sum_{k=1}^{n} a_k \cos kx_1 \Big\}$$

$$\mathcal{G}_n(\Gamma) = \big\{ g \in \mathrm{H}^{-1/2}(\Gamma) \,\big|\, \langle g, v\rangle = 0 \text{ for any } v \in \mathcal{S}_n(\Gamma) \big\},$$

then as in Section 2 we define

$$\Xi(\mathcal{S}_n, l) = \sup_h \|u(h)\|_{E(\Omega_l)}, \quad h \in \mathcal{G}_n, \ \|h\|_{\mathrm{H}^{-1/2}(\Gamma)} = 1.$$

To get lower estimate for Ξ, we will analyze a special class Υ of $\mathbf{A}$,

$$\begin{aligned} &\mathbf{A} = \{a_{i,j}\}, \quad i,j = 1,2, \\ &a_{1,1}(x) = c_1(x_1), \quad a_{2,2}(x) = c_2(x_1), \quad a_{1,2}(x) = a_{2,1}(x) = 0 \end{aligned} \tag{4.5}$$

where

$$c_1(x_1) = \frac{1}{\varphi'(x_1)}, \quad c_2(x_1) = \varphi'(x_1), \quad \varphi'(x_1) = d\varphi(x_1)/dx_1, \tag{4.6a}$$

$$0 < \alpha_0 \le \varphi'(x_1) \le \alpha_1 < \infty \tag{4.6b}$$

$$\varphi(-\pi) = -\pi, \quad \varphi(\pi) = \pi, \quad \varphi(x_1) \text{ is antisymmetric.} \tag{4.6c}$$

The function φ is a one to one mapping of $(-\pi,\pi)$ onto $(-\pi,\pi)$. Let

$$\xi = \varphi(x_1), \quad x_1 = \psi(\xi), \tag{4.7}$$

with

$$dx_1/d\xi = 1/\varphi'(x_1).$$

We have now

LEMMA 4.1. *Let $u_0(x_1,x_2)$ be the solution of the periodic Neumann problem with $\mathbf{A}(x)$ given in (4.5) and the boundary condition (4.2). Let*

$$w(\xi, x_2) = u_0(\psi(\xi), x_2), \tag{4.8}$$

then $w(\xi,x_2)$ is the solution of the periodic Neumann problem

$$\partial^2 w(\xi,x_2)/\partial\xi^2 + \partial^2 w(\xi,x_2)/\partial x_2^2 = \Delta w(\xi,x_2) = 0 \tag{4.9a}$$

$$\partial w/\partial x_2(\xi,0) = h(\psi(\xi))\psi'(\xi) \tag{4.9b}$$

$$\partial w/\partial x_2(\xi,q) = 0 \tag{4.9c}$$

and $\|w\|_{\mathrm{H}^1(\Omega)}$ is equivalent with $\|u_0\|_{E(\Omega)}$.

This lemma is easy to prove.

Let us prove

THEOREM 4.2. *There exists* $\mathbf{A}_n$ *of the form* (4.5), (4.6) *such that*

$$\Xi(\mathcal{S}_n, l) \geq C(l) n^{-1/2} \tag{4.10}$$

REMARK 4.1. In Theorem 4.2 the matrix $\mathbf{A}_n$ is dependent on n. A similar result for a special $\mathbf{A}$ independent of n will be proved in the sequel.

PROOF. Let

$$\cos\varphi(x_1) = \cos x_1 + \sigma(x_1), \tag{4.11}$$

where

$$\sigma(x_1) = \lambda \cos nx_1 \sin^4 x_1, \quad \lambda = O\left(\frac{1}{n}\right). \tag{4.12}$$

First we will prove that $\varphi(x_1)$ satisfies condition (4.6). We have

$$\varphi(x_1) = \arccos\big(\cos x_1 + \lambda \cos nx_1 \sin^4 x_1\big)$$

and $\varphi(x_1)$ is antisymmetric, $\varphi(-\pi) = -\pi$, $\varphi(\pi) = \pi$. For $x_1 \geq 0$ we get

$$\begin{aligned}\varphi'(x_1) = {} & \big(\sin x_1 + \lambda\big(n \sin nx_1 \sin^4 x_1 - 4\cos nx_1 \sin^3 x_1 \cos x_1\big)\big) \\ & \times \big(1 - \big(\cos x_1 + \lambda \cos nx_1 \sin^4 x_1\big)^2\big)^{-1/2}\end{aligned}$$

and

$$\begin{aligned}1 - & \big(\cos x_1 + \lambda \cos nx_1 \sin^4 x_1\big)^2 \\ & = \sin^2 x_1 \big(1 - 2\lambda \cos x_1 \cos nx_1 \sin^2 x_1 - \lambda^2 \cos^2 nx_1 \sin^6 x_1\big)\end{aligned}$$

and

$$\varphi'(x_1) = \frac{\big(1 + \lambda\big(n \sin x_1 \sin^3 x_1 - 4\cos nx_1 \sin^2 x_1 \cos x_1\big)\big)}{\big(1 - 2\lambda \cos x_1 \cos nx_1 \sin^2 x_1 - \lambda^2 \cos^2 nx_1 \sin^6 x_1\big)^{1/2}}.$$

Hence (4.6) holds for $\lambda = \frac{c}{n}$ with c sufficiently small and independent of n.

Let

$$W(\xi) = h(\psi(\xi))\psi'(\xi) = \partial w/\partial x_2(\xi, 0),$$

then $W(\xi) \in \mathrm{H}^{-1/2}(\Gamma)$ and

$$W(\xi) = \sum_{k=1}^{\infty} z_k \cos k\xi, \quad \pi \sum_{k=1}^{\infty} z_k^2 k^{-1} = \|W\|^2_{\mathrm{H}^{-1/2}(\Gamma)}.$$

Hence we have

$$w(\xi, x_2) = \sum_{k=1}^{\infty} z_k \cos k\xi \chi_k(x_2) k^{-1}$$

with

$$\chi_k = (e^{-kx_2} - e^{k(-2d+x_2)})/(1 - e^{-2kd})$$

and

$$\|w(\xi, x_2)\|_{\mathrm{H}^1(\Omega_l)} \geq |z_1| c(l).$$

We have

$$\begin{aligned} z_1 &= \pi^{-1} \int_{-\pi}^{\pi} \cos\xi \partial w/\partial x_2(\xi, 0) d\xi = \pi^{-1} \int_{-\pi}^{\pi} \cos\xi h(\psi(\xi))\psi'(\xi) d\xi \\ &= \pi^{-1} \int_{-\pi}^{\pi} h(x_1) \cos\varphi(x_1) dx_1 \\ &= \pi^{-1} \int_{-\pi}^{\pi} h(x_1) \cos x_1 dx_1 + \pi^{-1} \int_{-\pi}^{\pi} \sigma(x_1) h(x_1) dx_1. \end{aligned}$$

Further we have

$$\begin{aligned} &\cos nx_1 \sin^4 x_1 \\ &\quad = \frac{1}{16}(\cos(n+4)x_1 + \cos(n-4)x_1 - 4(\cos(n+2)x_1 \cos(n-2)x_1) \\ &\qquad + \frac{3}{8} \cos nx_1. \end{aligned} \tag{4.13}$$

Let $h(x_1) = \cos nx$. Then

$$|z| = C\lambda = O\left(\frac{1}{n}\right), \quad \text{and} \quad \|u_0\|_{\mathrm{H}^1(\Omega)} \geq O\left(\frac{1}{n}\right) \quad \text{with } \|h\|_{\mathrm{H}^{-1/2}(\Gamma)} = O\left(\frac{1}{n^{1/2}}\right)$$

which leads to (4.10) □

In Theorem 4.2 the matrix $\mathbf{A}$ depends on n. We now prove a similar theorem for a special coefficient matrix $\mathbf{A}$ that is chosen independently of n.

THEOREM 4.3. *There exist $h \in \mathrm{H}^{-1/2}(\Gamma)$ and a matrix $\mathbf{A}$ of the form* (4.5), (4.6) *such that*

$$\lim_{n\to\infty} \sup \Xi(\mathcal{S}_n, h)/n^{-1/2} \lg^5 n \geq C\|h\|_{\mathrm{H}^{-1/2}(\Gamma)}. \tag{4.14}$$

PROOF. Let

$$h(x_1) = \sum_{k=1}^{\infty} a_k \cos kx_1,$$

with

$$\begin{aligned} a_k &= \lg^{-2} k \quad \text{for } k = 2+9n,\ n = 1,2,\dots \\ &= 0 \qquad\quad\ \text{for } k \neq 2+9n,\ n = 1,2,\dots \end{aligned}$$

Define

$$b_k = a_k k^{-1/2},$$

then

$$\|h\|^2_{\mathrm{H}^{=1/2}(\Gamma)} = \pi \sum_{n=1}^{\infty} b_k^2 = \sum_{n=2}^{\infty} ((2+9n)\lg^4(2+9n))^{-1} \tag{4.15}$$

and

$$Q^2 = \sum_{n=1}^{\infty} b_k^2 \lg^2 k = \sum_{n=1}^{\infty} ((2+9n)\lg^2(2+9n))^{-1}. \tag{4.16}$$

Because (4.15) and (4.16) there exists a Rademacher function r (see [12, p. 205]), $r(k) = 1$ or -1, $k = 1,2,\dots$ such that

$$\rho(x_1) = \sum_{k=1}^{\infty} b_k r(k) \sin kx_1 = \sum_{k=1}^{\infty} b_k^* \sin kx_1$$

is a bounded function with

$$|\rho(x_1)| \leq CQ. \tag{4.17}$$

Further let

$$h^*(x_1) = \sum_{k=1}^{\infty} a_k r(k) \cos kx_1 = \sum_{k=1}^{\infty} a_k^* \cos kx_1$$

with

$$\|h^*\|_{\mathrm{H}^{-1/2}(\Gamma)} = \|h\|_{\mathrm{H}^{-1/2}(\Gamma)}.$$

Further let

$$\kappa(x_1) = \sum_{k=1}^{\infty} b_k^* k^{-1} \cos kx_1$$

then

$$\|d\kappa(x_1)/dx_1\|_{L^\infty(\Gamma)} = \|\rho(x_1)\|_{L^\infty(\Gamma)} \leq CQ. \tag{4.18}$$

Now analogously as before we let

$$\sigma(x_1) = \lambda\kappa(x_1)\sin^4 x_1 \tag{4.19}$$

and

$$\varphi(x_1) = \arccos(\cos x_1 + \sigma(x_1))$$

The inequalities (4.6) hold on noting that $\lambda = O(1)$ in (4.18).

Now we have

$$z_1 = \pi^{-1} \int_{-\pi}^{\pi} h^*(x_1)\sigma(x_1)dx_1 = \sum_{n=1}^{\infty}(\lg^{-4}(2+9n))(2+9n)^{-3/2} \tag{4.20}$$

where we have used the fact that $\langle h^*, \mathcal{S}_n\rangle = 0$.

From (4.20) we get

$$|z_1| \geq C(n+1)^{-1/2} \lg^{-5}(n+1)$$

and we obtain (4.14). □

In this analysis we have studied the penetration function associated with Neumann boundary data. However these results apply to Dirichlet boundary data noting that the Dirichlet problem can be transformed to the Neumann problem using the usual duality formulation.

The lower estimate was analyzed by considering an example given by a very special matrix $\mathbf{A}$. At this stage it is not yet clear what to expect for a general coefficient matrix. The example indicates that the upper estimate may be unduly pessimistic. We also have assumed that the $u \in \mathrm{H}^1(\Omega)$ only. Nevertheless it is known that u enjoys higher regularity and is Hölder continuous (see e.g., [13, 28]). Presently it is not clear how much this information could influence the decay rate for the penetration function with respect to n.

Obviously the penetration function depends on the class Υ. If we would consider the class of problems with $\mathbf{A} \in \mathrm{H}^{k,\infty}(\Omega)$ then $u \in \mathrm{H}^{k+1}$ and the lower estimate can be obtained in an analogous way. There is a practical difficulty with the characterization of the class Υ, for example when considering fiber reinforced composite materials (see [4]), the fibers have circular cross-section with the diameter $d \sim 7\mu$. Regularity theory shows that the solution u is an element of $H^{3/2-\epsilon}(\Omega)$, however the associated norm is very large. So practically it is better to view the solution u as an element of $H^{1/2}(\Omega)$ where the norm is of reasonable size.

There are many open problems related to the penetration function. In the next section we will provide a numerical approach for determining the penetration function associated with the class Υ_0 of matrices $\mathbf{A}$ with coefficients taking only two values.

5 The penetration function for piece-wise constant coefficients.

In the first part of this section we show that the lower bound on the penetration function given in Theorem 4.2 applies to the class Υ_0 for special choices of γ_1 and γ_2. In the second part we proceed directly and provide a numerical method for computing lower bounds on the penetration function for the class Υ_0. We use the method to compute lower bounds on the Neuman penetration function for different choices of γ_1 and γ_2. The results of the computations are used to estimate the decay of the penetration function as a function of γ_1 and γ_2.

5.1 Correspondence between Υ_0 and the coefficient matrices of Section 4.

Recall the class Υ_0 of matrices $\mathbf{A}$ with coefficients taking only two values given in the introduction. Matrices in this class are written as

$$\mathbf{A} = \gamma(x)\mathbf{I} \tag{5.1}$$

where $\gamma(x)$ is any simple function taking only the values γ_1 or γ_2. We emphasize the dependence on γ_1 and γ_2 and write this class as $\Upsilon_0(\gamma_1, \gamma_2)$. The set of all G-limits (H-Limits) associated with this class is well known [33, 21]. This set of coefficient matrices is referred to as the G-closure of $\Upsilon_0(\gamma_1, \gamma_2)$ [21] and we denote it by $G\Upsilon_0(\gamma_1, \gamma_2)$. It is also known that every coefficient matrix in $G\Upsilon_0(\gamma_1, \gamma_2)$ is realized by the effective coefficient matrices of G-convergent sequences of simple functions associated with layered configurations [33, 21]. The effective coefficient matrices $\mathbf{A}^L$ associated with these limits are of the form $\mathbf{A}^L = \mathbf{R}^T(\beta)\mathbf{C}\mathbf{R}(\beta)$ where $\mathbf{R}(\beta)$ is a rotation matrix associated with a rotation of β radians and the diagonal matrix $\mathbf{C}$ is given by

$$\mathbf{C} = \begin{bmatrix} c_1 & 0 \\ 0 & c_2 \end{bmatrix}, \tag{5.2}$$

with coefficients given by

$$\begin{aligned} c_1(\theta, \rho) &= \gamma_1 + \frac{\theta\gamma_1(\gamma_2 - \gamma_1)}{\gamma_1 + (1-\theta)(1-\rho)(\gamma_2 - \gamma_1)} \\ c_2(\theta, \rho) &= \gamma_1 + \frac{\theta\gamma_1(\gamma_2 - \gamma_1)}{\gamma_1 + (1-\theta)\rho(\gamma_2 - \gamma_1)}, \end{aligned} \tag{5.3}$$

where θ, ρ and β are measurable functions and $\theta = \theta(x)$ is the local area fraction of γ_2, $\rho = \rho(x)$ is the local anisotropy parameter, and $\beta = \beta(x)$ is the local layer orientation with

$$0 \le \theta \le 1, \quad 0 \le \rho \le 1, \quad 0 \le \beta \le \pi. \tag{5.4}$$

THEOREM 5.1. *There exist fixed choices γ_1 and γ_2 independent of $n = 1, 2 \ldots$ such that for every matrix $\mathbf{A}_n$ defined in Theorem 4.2 there is a diagonal matrix $\mathbf{A}_n^L$ of the form $\mathbf{A}_n^L = \mathbf{C}$ with $\mathbf{C}$ given by* (5.2) *and* (5.3) *such that*

$$\mathbf{A}_n = \mathbf{A}_n^L. \tag{5.5}$$

PROOF. Solution of the system $c_1(\theta, \rho) = 1/\varphi'$, $c_2(\theta, \rho) = \varphi'$ shows that the resulting curve $\theta = \theta(\varphi')$, $\rho = \rho(\varphi')$ satisfies the constraints (5.4) when γ_1 and γ_2

are chosen to satisfy the inequalities

$$\frac{\gamma_1^{-1} - \gamma_1 + \gamma_2 - \gamma_2^{-1}}{\frac{\gamma_2}{\gamma_1} - \frac{\gamma_1}{\gamma_2}} < \alpha_0 < \alpha_1 < \frac{\frac{\gamma_2}{\gamma_1} - \frac{\gamma_1}{\gamma_2}}{\gamma_1^{-1} - \gamma_1 + \gamma_2 - \gamma_2^{-1}} \tag{5.6}$$

and

$$\gamma_1 < 1 < \gamma_2. \tag{5.7}$$

Here the first inequality (5.6) follows from the well known harmonic mean – arithmetic mean bounds on c_1 and c_2 while (5.7) is necessary for the curve $c_1^{-1} = c_2$ to lie in the set $G\Upsilon_0(\gamma_1, \gamma_2)$. □

For future reference we display the curves for θ and ρ. These are given by

$$\theta = \frac{(\gamma_1 + \gamma_2)\big(1 - \varphi'\gamma_1\big)\big(\varphi' - \gamma_1\big)}{\varphi'\big(1 - \gamma_1^2\big)(\gamma_2 - \gamma_1)} \tag{5.8}$$

$$\rho = 1 + \gamma_1\left(\frac{\varphi'\big(1 - \gamma_1^2\big) - (\gamma_1 + \gamma_2)\big(1 - \varphi'\gamma_1\big)}{\varphi'(\gamma_2 - \gamma_1)\big(1 - \gamma_1^2\big) - (\gamma_1 + \gamma_2)\big(1 - \varphi'\gamma_1\big)\big(\varphi' - \gamma_1\big)}\right). \tag{5.9}$$

The penetration function for a generic class of coefficients Υ is defined to be the supremum of $\Xi(\mathcal{S}_n, l)$ taken over all coefficient matrices in that class. The supremum is denoted by $\Xi(\mathcal{S}_n, l, \Upsilon)$. The associated penetration function for the class $\Upsilon_0(\gamma_1, \gamma_2)$ is written $\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2))$. Theorem 5.1 enables one to apply the lower bound displayed in Theorem 4.2 to $\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2))$. This is expressed in the following theorem.

THEOREM 5.2. *Given that γ_1 and γ_2 satisfy* (5.6) *and* (5.7) *then the penetration function for the class $\Upsilon_0(\gamma_1, \gamma_2)$ satisfies*

$$\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2)) \geq C(l) n^{-1/2}. \tag{5.10}$$

PROOF. For each coefficient matrix $\mathbf{A}_n$ given in Theorem 4.2 one applies Theorem 5.1 to assert the existence of a sequence of coefficient matrices $\{\gamma_k(x)\mathbf{I}\}_{k=1}^{\infty}$ in $\Upsilon_0(\gamma_1, \gamma_2)$ associated with locally layered configurations that G-converge to $\mathbf{A}_n^L = \mathbf{A}_n$. The corresponding solutions of (1.1) with $\mathbf{A} = \gamma_k(x)\mathbf{I}$ are denoted by u_k. Theorem 5.2 then follows noting that the energies $\int_{\Omega_l} (\nabla u_k)^T \gamma_k(x) \mathbf{I} (\nabla u_k) dx$ converge to the limit energy associated with $\mathbf{A}_n$. □

5.2 A numerical method for computing the decay of the penetration function and applications.

The calculation of $\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2))$ is a problem of optimal design and requires one to take a supremum of an objective function over the class of simple functions. This type of problem is well known to be theoretically ill-posed over the class $\Upsilon_0(\gamma_1, \gamma_2)$ see, [23, 19]. The problem is made well-posed by noting that the objective function is continuous with respect to G-convergence and extending the class $\Upsilon_0(\gamma_1, \gamma_2)$ to include the set of G-limits $G\Upsilon_0(\gamma_1, \gamma_2)$ associated with all G-convergent sequences of coefficient matrices in $\Upsilon_0(\gamma_1,\gamma_2)$. This fact can be stated as

$$\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2)) = \Xi(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1,\gamma_2)). \tag{5.11}$$

The set $G\Upsilon_0(\gamma_1,\gamma_2)$ is known explicitly and can be parameterized using the explicit formulas for $\mathbf{A}^L$ given in the previous section, see, [21, 33]. This theory is now well known and was introduced in [20, 24]. With this theory in hand one can write

$$\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2)) = \sup_{(\theta,\rho,\beta)} \left\{\Xi(\mathcal{S}_n, l), \mathbf{A}^L = \mathbf{R}^T(\beta)\mathbf{C}\mathbf{R}(\beta)\right\}, \tag{5.12}$$

with $\mathbf{C}$ defined by (5.2) and (5.3) and the parameters θ, ρ, and β subject to the box constraints (5.4). Here the supremum on the right hand side of (5.12) can be computed numerically.

In view of future applications we point out that penetration functions can also be defined in terms of $\|\nabla u(h)\|_{L^2(\Omega_l)}$. For this case put

$$\mathcal{P}(\mathcal{S}_n, l) = \sup_h \|\nabla u(h)\|_{L^2(\Omega_l)}, \quad h \in \mathcal{G}_n, \quad \|h\|_{\mathrm{H}^{-1/2}(\Gamma)} = 1, \tag{5.13}$$

and the penetration function $\Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2))$ for the class $\Upsilon_0(\gamma_1,\gamma_2)$ is equivalent to the penetration function $\mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2))$ defined by

$$\mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2)) = \sup_{\mathbf{A}}\{\mathcal{P}(\mathcal{S}_n, l), \mathbf{A} \in \Upsilon_0(\gamma_1,\gamma_2)\}. \tag{5.14}$$

Here it is easily seen that

$$\sqrt{\gamma_1}\mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2)) \leq \Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2)) \leq \sqrt{\gamma_2}\mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2)). \tag{5.15}$$

In the following simulations we work with the penetration function given by (5.14). The evaluation of $\mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1,\gamma_2))$ is also an ill-posed problem of optimal design. To make the problem well posed we: 1) extend the class $\Upsilon_0(\gamma_1,\gamma_2)$ to $G\Upsilon_0(\gamma_1,\gamma_2)$ and 2) identify all limit points of the sequences $\{\|\nabla u_n(h)\|_{L^2(\Omega_l)}\}_{n=1}^{\infty}$ associated with G-convergent sequences $\{\mathbf{A}_n\}_{n=1}^{\infty} \in \Upsilon_0(\gamma_1,\gamma_2)$. These limits are identified in [17, 18] and are given by

$$\lim_{n\to\infty} \|\nabla u_n(h)\|_{L^2(\Omega_l)} = \left(\int_{\Omega_l} (\nabla u_H)^T(\partial_{\gamma_1}\mathbf{A}_H + \partial_{\gamma_2}\mathbf{A}_H)(\nabla u_H)dx\right)^{1/2} \tag{5.16}$$

where $\mathbf{A}_H$ is the G-limit of the sequence, u_H is the homogenized solution and ∂_{γ_1} and ∂_{γ_2} are the derivatives of $\mathbf{A}_H$ with respect to the parameters γ_1 and γ_2.

In order to proceed with the numerical computation of lower bounds on the penetration function we incorporate the explicit parameterization of the set of G-limits given by the coefficient matrices $\mathbf{A}^L$ and write

$$\mathcal{R}(u(h)) = \left(\int_{\Omega_l} (\nabla u(h))^T\left(\partial_{\gamma_1}\mathbf{A}^L + \partial_{\gamma_2}\mathbf{A}^L\right)(\nabla u(h))dx\right)^{1/2} \tag{5.17}$$

where $u(h)$ solves (1.1) with $\mathbf{A} = \mathbf{A}^L$. We put

$$\mathcal{RP}(\mathcal{S}_n, l) = \sup_h \mathcal{R}(u(h)), \quad h \in \mathcal{G}_n,\ \|h\|_{\mathrm{H}^{-1/2}(\Gamma)} = 1, \tag{5.18}$$

and define the relaxed penetration function $\mathcal{RP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2))$ given by

$$\mathcal{RP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2)) = \sup_{(\theta,\rho,\beta)} \left\{\mathcal{R}(\mathcal{S}_n, l), \mathbf{A}^L = \mathbf{R}^T(\beta)\mathbf{C}\mathbf{R}(\beta)\right\}, \tag{5.19}$$

with $\mathbf{C}$ defined by (5.2) and (5.3) and the parameters θ, ρ, and β subject to the box constraints (5.4). It is shown in [5] that

$$\mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2)) = \mathcal{RP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2)). \tag{5.20}$$

A lower bound is obtained by fixing $h_n = a_n \cos{(n+1)x}$ in $\mathcal{G}_n$ with $\|h_n\|_{\mathrm{H}^{-1/2}(\Gamma)} = 1$, and computing

$$\mathcal{LP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2)) = \sup_{(\theta,\rho,\beta)} \left\{\mathcal{R}(u(h_n)), \mathbf{A}^L = \mathbf{R}^T(\beta)\mathbf{C}\mathbf{R}(\beta)\right\}. \tag{5.21}$$

Then

$$\mathcal{LP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2)) \leq \mathcal{P}(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2)) \tag{5.22}$$

and from (5.15)

$$\sqrt{\gamma_1}\mathcal{LP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2)) \leq \Xi(\mathcal{S}_n, l, \Upsilon_0(\gamma_1, \gamma_2)). \tag{5.23}$$

The lower bound $\mathcal{LP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2))$ is computed using the solutions of (1.1a) on the strip Ω defined in Section 4. Here the strip is of width 1, i.e., $q = 1$. In the computations the non-homogeneous Neuman boundary condition (4.2b) is given by $h_n = a_n \cos nx_1$. This boundary condition is applied to the top of the strip $x_1 \in \Gamma$, $x_2 = 1$. The homogeneous Neuman boundary condition is applied on the bottom of the strip, $x_1 \in \Gamma$, $x_2 = 0$. For these examples Ω_l, $l = 1/2$, is the bottom half of the strip $\{x|\, x_1 \in \Gamma,\ 0 < x_2 < 1/2\}$. The distance separating the inhomogeneous boundary data and Ω_l is $1/2$. We carry out the optimization over the design parameters θ, ρ, β using a steepest decent method.

We compute the lower bound $\mathcal{LP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2))$ for $n = 1, \ldots, 100$ for the choices $\gamma_1 = 1.0$, $\gamma_2 = 10$ and $\gamma_1 = 0.5$, $\gamma_2 = 10$. The plots of $\lg(n)$ versus $\lg(\mathcal{LP}(\mathcal{S}_n, l, G\Upsilon_0(\gamma_1, \gamma_2)))$ are the upper two curves displayed in Figure 5.1. The top curve corresponds to $\gamma_1 = 0.5$, $\gamma_2 = 10$ and the one below corresponds to $\gamma_1 = 1.0$, $\gamma_2 = 10$. Both of these curves flatten out with increasing n and are seen to decay at a rate of $n^{-0.4}$. The lowest curve in Figure 5.1 corresponds to the lower bound on the decay of the penetration function given by $\mathcal{R}(h_n)$ associated with $\mathbf{A}_n$ given in Theorem 4.2 with $\lambda = 0.44/n$ in (4.12). For each $\mathbf{A}_n$ we equate it with a G-limit according to Theorem 5.1. Here the G-limit is associated with a sequence of simple functions taking the values $\gamma_1 = 0.5$ and $\gamma_2 = 10$. It is seen that the lowest curve decays as $n^{-1/2}$.

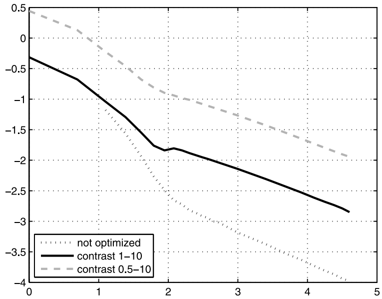

Figure 5.1: Decay of the penetration function.

The local area fraction θ of γ_2 corresponding to the optimal design attaining $\mathcal{LP}(\mathcal{S}_5, l, G\Upsilon_0(\gamma_1, \gamma_2))$ with $\gamma_1 = 0.5, \gamma_2 = 10$ is plotted in Figure 5.2. Here $\theta = 0$ inside the white region, $\theta = 1$ in the black regions, and θ takes values between zero and one in the gray regions. The coefficient matrix associated with θ takes the value $\gamma_2\mathbf{I}$ in the black regions, the value $\gamma_1\mathbf{I}$ in the white region, and the gray zone corresponds to the G-limit (effective coefficient) associated with the local microstructure. The local flux field $j = \mathbf{A}^L\nabla u(h_5))$ and level curves of $u(h_5)$ associated with the optimal design are plotted in Figure 5.3.

It is also interesting to compare the designs that generate data points on the highest and lowest curves in Figure 5.1. The local area fraction of material two associated with $\mathbf{A}_{10}$ is plotted in Figure 5.4. This coefficient matrix was

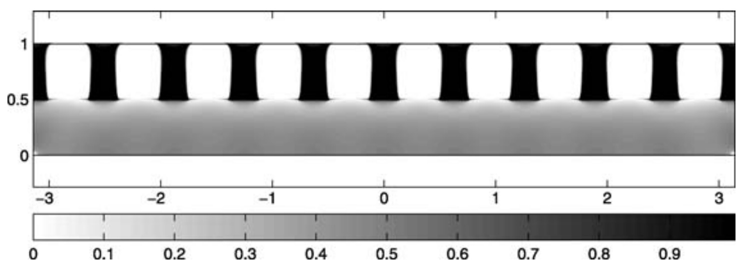

Figure 5.2: Area fraction distribution inside the optimal design for $n = 5$.

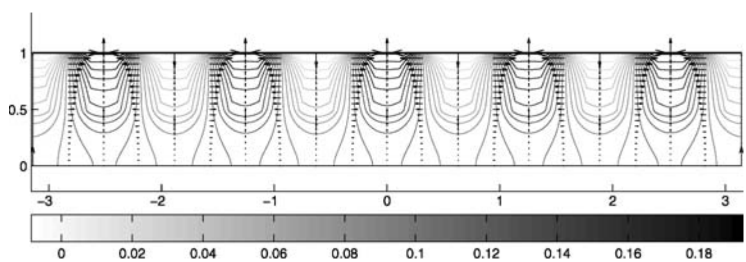

Figure 5.3: Vectors indicate local flux fields plotted with level curves of u, inside the optimal design for $n = 5$.

used to generate the data point for the choice $n = 10$ on the lowest curve in Figure 5.1. The data point for the choice $n = 10$ lying on the highest curve in Figure 5.1 corresponds to an optimized design. The local area fraction of material two for this design is plotted in Figure 5.5 for comparison. The design in Figure 5.4 corresponds to one in which the coefficient matrix is changing in the x_1 coordinate only. While the design in Figure 5.5 is optimized over all coefficients in the class $\Upsilon_0(\gamma_1, \gamma_2)$ and exhibits variation along both the x_1 and x_2 directions.

In Figure 5.6 we display the normalized lower bounds on the penetration function for $\gamma_1 = 1$, $\gamma_2 = 10$ and $\gamma_1 = 0.5$, $\gamma_2 = 10$. Here the bounds are normalized so that the bounds equal one for $n = 1$. Comparison of the curves show that the curve corresponding to the higher contrast case $\gamma_1 = 0.5$, $\gamma_2 = 10$ lies above

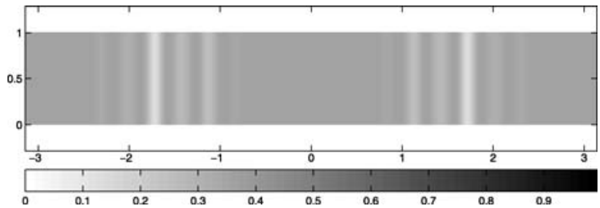

Figure 5.4: Area fraction distribution inside a design for $n = 10$ corresponding to class of matrices in Theorem 4.1.

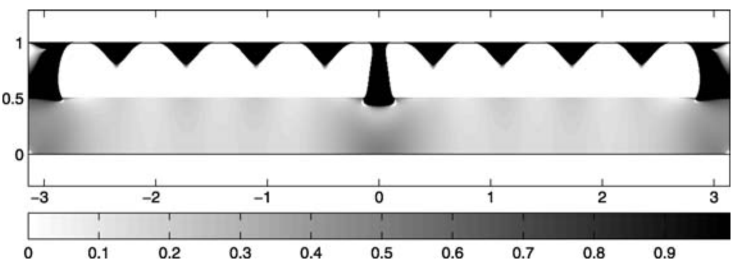

Figure 5.5: Area fraction distribution inside the optimal design for $n = 10$.

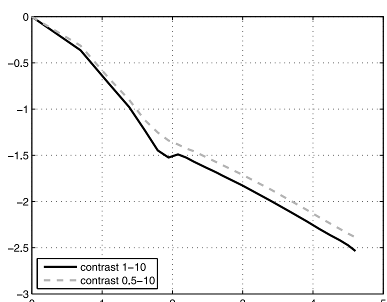

Figure 5.6: Decay of the normalized penetration function.

the curve corresponding to the lower contrast case $\gamma_1 = 1$, $\gamma_2 = 10$. However the slopes of the curves remain nearly the same for larger values of n. This behavior is surprising in view of the upper bound on the penetration function presented in Section 3 which becomes significantly flatter with an increase in the contrast γ_2/γ_1.

REFERENCES

1. A. Abdulle and B. Engquist, *Finite element heterogeneous multiscale methods with near optimal computational complexity*, Isaac Newton Institute for Mathematical Sciences, preprint, NI0746-HOP, 2007.
2. I. Babuška, *Homogenization and its applications, mathematical and computational problems*, in Numerical Solution of Partial Differential Equations III (SYNSPADE 1975, Maryland, May 1975), B. Hubbard, ed., Academic Press, New York, 1976, pp. 89–110.
3. I. Babuška, G. Calosh, and J. Osborn, *Special finite element method for a class of second order elliptic problems with rough coefficients*, SIAM J. Numer. Anal., 31 (1994), pp. 945–981.
4. I. Babuška, B. Andersson, P. J. Smith, and K. Levin, *Damage analysis of fiber composites, part I statistical analysis on fiber scale*, Comput. Methods Appl. Mech. Eng., 172 (1999), pp. 27–78.
5. I. Babuška, R. Lipton, and M. Stüebner, *A generalization of Saint Venant's principle and applications of penetration functions*, preprint.
6. A. Bensoussan, J. L. Lions, and G. C. Papanicolau, *Asymptotic Analysis for Periodic Structures*, North-Holland, Amsterdam, 1978.
7. M. Biroli and U. Mosco, *A Saint-Venant type principle for Dirichlet forms on discontinuous media*, Ann. Math. Pure Appl. (IV), CLXIX (1995), pp. 125–181.
8. T. Breitzman, R. Lipton, and E. Iarve, *Local field assessment inside multiscale composite architectures*, SIAM Multiscale Model. Simul., 6 (2007), pp. 937–962.
9. V. Buriachenko, *Micromechanics of Heterogenous Materials*, Springer, New York, 2007.
10. W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden, *Heterogeneous multiscale methods: A review*, Commun. Comput. Phys., 2 (2007), pp. 367–450.
11. W. E, P. Ming and P. Zhang, *Analysis of the heterogeneous multiscale method for elliptic homogenization problems*, J. Am. Math. Soc, 18 (2005), pp. 1544–1585.
12. R. E. Edwards, *Fourier Series, A Modern Introduction, Vol. II*, Holt, Rinehard, and Winston, Inc., New York, 1967.
13. D. Gilbarg and N. S. Trudinger, *Elliptic Partial Differential Equations of Second Order*, Springer, New York, 1998.
14. T. Y. Hou and X. H. Wu, *A multiscale finite element method for elliptic problems in composite material and porous media*, J. Comput. Phys., 134 (1997), pp. 169–189.
15. V. V. Jikov, S. M. Kozlov, and O. A. Oleinik, *Homogenization of Differential Operators and Integral Functionals*, Springer, New York, 1994.
16. A. Kufner, *Weighted Sobolev Spaces*, J. Wiley & Sons, Hoboken, NJ, 1985.
17. R. Lipton, *Relaxation through homogenization for optimal design problems with gradient constraints*, J. Optimization Theory Appl., 114 (2002), pp. 27–53.
18. R. Lipton, *Assessment of the local stress state through macroscopic variables*, Proc. R. Soc. Lond., Ser. A, Math. Phys. Eng. Sci., 361 (2003), pp. 921–946.
19. K. A. Lurie, *On the optimal distribution of the resistivity tensor of the working substance in a magnetohydrodynamic channel*, J. Appl. Math. Mech., 34 (1970), pp. 255–274.

20. K. A. Lurie, and A. V. Cherkaev, *Effective characteristics of composite materials and the optimal design of structural elements*, Usp. Mekh., Adv. Mech., 9 (1986), pp. 3–81, (English translation in Topics in the Mathematical Modelling of Composite Materials, A. V. Cherkaev and R. V. Kohn, eds., Progr. Nonlinear Differ. Equations Appl., vol. 31, Birkhäuser, Boston, 1997, pp. 175–258.).

21. K. A. Lurie and A. V. Cherkaev, *Exact estimates of conductivity of mixtures composed of two materials taken in prescribed proportion (plane problem)*, Dokl. Akad. Nauk SSSR, 264 (1982), pp. 1128–1130.

22. V. Mazja, M. Mitrea, and T. Shaposhnikova, *The Dirichlet problem in Lipschitz domains for higher order elliptic systems with rough coefficients*, preprint.

23. F. Murat, *Un contre-example pour le problème du contrôle dans les coefficients*, C. R. Acad. Sci., Paris, Sér. A, 273 (1971), pp. 708–711.

24. F. Murat and L. Tartar, *Calcul des variations et homogénéisation*, in Les Méthodes de l'Homogénéisation: Théorie et Applications en Physique, D. Bergman, J. L. Lions, and G. Papanicolaou, eds., Collection de la Direction des Études et Recherches d'Electricité de France, vol. 57, Eyrolles, Paris, 1985, pp. 319–369, (English translation: F. Murat and L. Tartar, *Calculus of variations and homogenization*, in Topics in the Mathematical Modelling of Composite Materials, A. V. Cherkaev and R. V. Kohn, eds., Progr. Nonlinear Differ. Equations Appl., vol. 31, Birkhäuser, Boston, 1997, pp. 139–173.).

25. F. Murat, *H-convergence*, in Séminaire d'Analyse Fonctionelle et Numérique de l'Université d'Alger, 1978, mimeographed notes, (Translated into English as F. Murat and L. Tartar, *H-convergence*, in Topics in the Mathematical Modelling of Composite Materials, A. V. Cherkaev and R. V. Kohn, eds., Progr. Nonlinear Differ. Equations Appl., vol. 31, Birkhäuser, Boston, 1997, pp. 21–43.).

26. J. Nečas, *Sur une methode pour resoudre les equations aux derivees partielles du type elliptique voisine de la variatinnelle*, Ann. Sc. Norm. Super. Pisa, 16 (1962), pp. 305–326.

27. J. T. Oden and K. S. Vegemanti, *Estimation of local modeling error and global-oriented adaptive modeling of heterogenous materials: error estimates and adaptive algorithms*, J. Comput. Phys., 164 (2000), pp. 22–47.

28. L. C. Piccinini and S. Spagnolo, *On Hölder continuity of solutions of second order elliptic equations in two variables*, Ann. Sc. Norm. Pisa, 26 (1972), pp. 391–402.

29. A. Pinkus, *n-Width in Approximation Theory*, Springer, New York, 1985.

30. S. Spagnolo, *Convergence in energy for elliptic operators*, in Numerical Solution of Partial Differential Equations III, B. Hubbard, ed., Academic Press, New York, 1976, pp. 469–498.

31. T. Strouboulis, L. Zhang, and I. Babuška, *p-version of generalized FEM using mesh-based handbooks with applications to multiscale problems*, Int. J. Numer. Methods Eng., 60 (2004), pp. 1639–1672.

32. T. Strouboulis, L. Zhang, and I. Babuška, *Generalized finite element method using mesh-based handbooks: application to problems in domains with many voids*, Comput. Methods Appl. Mech. Eng., 192 (2003), pp. 3109–3161.

33. L. Tartar, *Estimations fines de coefficients homogénéisés*, in Ennio De Georgi Colloquium, P. Kree, ed., Res. Notes Math., vol. 125, Pitman, London, 1985, pp. 168–187.