High-accuracy approximation of effective coefficients

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Summary. In this contribution we study the calculation of effective coefficients for media with periodic heterogeneities. We use finite element methods of high order which allows to obtain high accuracy with relatively low computational effort. This is shown both theoretically and practically.

Key words: Homogenisation, partial differential equations, multigrid, domain decomposition, preconditioning.

1 Introduction

When simulating heterogeneous media, it is often impossible to simulate the microscopic processes directly. Instead, it is necessary to fall back on so-called homogenised models, which describe the behaviour of a reduced representation of the solution, usually obtained by some kind of averaging procedure. Depending on the smallness of the ratio between the microscopic and macroscopic scale, the error of the homogenised model tends to zero, and often it is a completely satisfactory way to formulate the problem under consideration. If sufficient information about the microstructure is available, the effective properties of the medium can be calculated by solving suitable problems on representative cells and averaging.

In this article, we restrict ourselves to the special case of periodic heterogeneities occurring in two model systems of partial differential equations, namely linear elasticity and Stokes flow. After introducing the model problems, the homogenisation process is described including convergence results and error estimates. Finally, numerical results are presented in Section 5.

2 Model problems

This section introduces the two model problems considered in this article. The first problem is linear elasticity with a heterogeneous coefficient, the second is Stokes flow through a porous domain.

Let us describe the first problem. Let $\mathbf{A} : \mathbb{R}^n \to (\mathbb{R}^{n\times n})^{n\times n}$ be a 4-tensor with 1-periodic components $\mathbf{A}_{ij}^{kl} \in L^\infty(\mathbb{R}^n, \mathbb{R})$. The tensor $\mathbf{A}$ can be chosen to satisfy for all $i, j, k, h \in \{1, \ldots, n\}$ the symmetry conditions

$$\mathbf{A}_{ij}^{hk}(y) = \mathbf{A}_{ji}^{kh}(y) = \mathbf{A}_{hj}^{ik}(y)\,,\ y \in \mathbb{R}^n\,, \tag{1}$$

and appropriate ellipticity and continuity are the existence of constants $0 < \lambda_1 \leq \lambda_2$ with

$$\lambda_1 \sum_{i,j=1}^{n} |\eta_{ik}|^2 \leq \mathbf{A}_{ij}^{hk}(y)\eta_{ih}\eta_{jk} \leq \lambda_2 \sum_{i,j=1}^{n} |\eta_{ik}|^2 \tag{2}$$

for all $y \in \mathbb{R}^n$ and all symmetric matrices $\eta \in \mathbb{R}^{n\times n}$.

First we introduce some notation for function spaces: for $\Omega \subset \mathbb{R}^n$ being a bounded Lipschitz domain, we denote with $L^2(\Omega)$ the set of all square-integrable functions, and set

$$L_0^2(\Omega) = \{u \in L^2(\Omega) : \textstyle\int_\Omega u(x)\,dx = 0\}\,, \tag{3}$$

$$H^1(\Omega) = \{u \in L^2(\Omega) : \nabla u \in L^2(\Omega, \mathbb{R}^n)\}\,, \tag{4}$$

$$H_0^1(\Omega) = \{u \in H^1(\Omega) : u = 0 \text{ on } \partial\Omega\}\,. \tag{5}$$

Spaces for vector-valued functions are denoted with $L^2(\Omega, \mathbb{R}^n) \cong (L^2(\Omega))^n$, $H^1(\Omega, \mathbb{R}^n) \cong (H^1(\Omega))^n$, etc.

Now the elasticity problem is the following: given $\mathbf{f} \in L^2(\Omega, \mathbb{R}^n)$, we search for $\mathbf{u}^\varepsilon \in H_0^1(\Omega, \mathbb{R}^n)$ such that

$$\mathbf{a}^\varepsilon(\mathbf{u}^\varepsilon, \mathbf{v}) := \int_\Omega \nabla\mathbf{v}(x) : (\mathbf{A}(\frac{x}{\varepsilon})\nabla\mathbf{u}^\varepsilon(x))\,dx = \int_\Omega \mathbf{f}(x)\cdot\mathbf{v}(x)\,dx \tag{6}$$

for all $\mathbf{v} \in H_0^1(\Omega, \mathbb{R}^n)$. Here, $a\cdot b$ denotes the Euclidean scalar product between vectors $a, b \in \mathbb{R}^n$, and $M : N = \operatorname{trace}(M^t N)$ generalises this scalar product to arbitrary rectangular matrices $M, N \in \mathbb{R}^{m\times n}$. Equation (6) is the variational form of the equation

$$\begin{aligned} -\operatorname{div}\left(\mathbf{A}(\frac{x}{\varepsilon})\nabla\mathbf{u}^\varepsilon(x)\right) &= \mathbf{f}(x)\,, \qquad x \in \Omega \\ \mathbf{u}^\varepsilon(x) &= 0\,, \qquad x \in \partial\Omega\,. \end{aligned} \tag{7}$$

Korn's inequality shows that the Lemma of Lax-Milgram is applicable and yields existence and uniqueness of $\mathbf{u}^\varepsilon \in H_0^1(\Omega, \mathbb{R}^n)$.

The second model problem is (generalised) Stokes flow in a medium with periodically distributed holes. Let $\Box = (0,1)^n$. For a smoothly bounded compact subset $\emptyset \neq Z \subset\subset \Box$, we set $Y = \Box - Z$ and

$$Z^\varepsilon = \bigcup_{\mathbf{k}\in\mathbb{Z}^n, \varepsilon(\mathbf{k}+\Box)\subset\Omega} \varepsilon(\mathbf{k}+Z)\,, \qquad \Gamma^\varepsilon = \partial Z^\varepsilon\,, \qquad \Omega^\varepsilon = \Omega \setminus Z^\varepsilon\,. \tag{8}$$

Given then $\mathbf{f}^\varepsilon \in L^2(\Omega^\varepsilon, \mathbb{R}^n)$ and $g^\varepsilon \in L^2_0(\Omega^\varepsilon)$, we search for a pair $(\mathbf{u}^\varepsilon, p^\varepsilon) \in H^1_0(\Omega^\varepsilon, \mathbb{R}^n) \times L^2_0(\Omega^\varepsilon)$ such that

$$\begin{aligned} \int_{\Omega^\varepsilon} \nabla\mathbf{u}^\varepsilon : \nabla\mathbf{v}\,dx - \int_{\Omega^\varepsilon} p^\varepsilon \operatorname{div}\mathbf{v}\,dx = \int_{\Omega^\varepsilon} \mathbf{f}^\varepsilon\cdot\mathbf{v}\,dx\,, \qquad \mathbf{v}\in H^1_0(\Omega^\varepsilon,\mathbb{R}^n)\,, \\ \int_{\Omega^\varepsilon} \operatorname{div}\mathbf{u}^\varepsilon\, q\,dx = \varepsilon^2 \int_{\Omega^\varepsilon} g^\varepsilon\, q\,dx\,, \qquad q\in L^2_0(\Omega)\,, \end{aligned} \tag{9}$$

which is the weak form of

$$\begin{aligned} -\Delta\mathbf{u}^\varepsilon(x) + \nabla p^\varepsilon(x) = \mathbf{f}^\varepsilon(x)\,, \qquad x\in\Omega^\varepsilon\,, \\ \operatorname{div}\mathbf{u}^\varepsilon(x) = \varepsilon^2 g^\varepsilon(x)\,, \qquad x\in\Omega^\varepsilon\,, \\ \mathbf{u}^\varepsilon(x) = 0\,, \qquad x\in\partial\Omega^\varepsilon\,. \end{aligned} \tag{10}$$

Theorem 1. *On Ω^ε, the Poincaré estimate*

$$\|\mathbf{u}^\varepsilon\|_{L^2(\Omega^\varepsilon)} \lesssim \varepsilon \|\nabla\mathbf{u}^\varepsilon\|_{L^2(\Omega^\varepsilon)} \tag{11}$$

is valid, and the Babuška-Brezzi stability constant satisfies

$$\beta_{\Omega^\varepsilon} = \inf_{0\neq q\in L^2(\Omega^\varepsilon)} \sup_{\mathbf{v}\in H^1_0(\Omega^\varepsilon,\mathbb{R}^n)} \frac{(\operatorname{div}\mathbf{v}, q)_{L^2(\Omega^\varepsilon)}}{\|q\|_{L^2(\Omega^\varepsilon)}\|\mathbf{v}\|_{H^1_0(\Omega^\varepsilon,\mathbb{R}^n)}} \gtrsim \varepsilon\,. \tag{12}$$

An immediate consequence is the a-priori estimate

$$\frac{1}{\varepsilon^2}\|\mathbf{u}^\varepsilon\|_{L^2(\Omega^\varepsilon)} + \frac{1}{\varepsilon}\|\nabla\mathbf{u}^\varepsilon\|_{L^2(\Omega^\varepsilon)} + \|p^\varepsilon\|_{L^2(\Omega)} \lesssim \|\mathbf{f}^\varepsilon\|_{L^2(\Omega^\varepsilon,\mathbb{R}^n)} + \|g^\varepsilon\|_{L^2(\Omega^\varepsilon)} \tag{13}$$

for solutions of (9) resp. (10).

Proof. Estimate (11) can easily be proved in each cell due to the Dirichlet condition on Γ^ε. Now we give a sketch of a proof for (12). For a given $q \in L^2_0(\Omega^\varepsilon)$, one has to construct a velocity field $\mathbf{v} \in H^1_0(\Omega^\varepsilon)$ such that $(\operatorname{div}\mathbf{v}, q)_{L^2(\Omega^\varepsilon)}$ is reasonably large. This is done as follows. First, one defines $\lambda \in H^1(\Omega)$ as solution to

$$\Delta\lambda(x) = q(x)\,, \qquad x\in\Omega^\varepsilon\,, \quad \frac{\partial\lambda}{\partial n} = 0\,, \qquad x\in\partial\Omega^\varepsilon\,.$$

Then $\mathbf{v}_1 := \nabla\lambda \in H^1(\Omega^\varepsilon, \mathbb{R}^n)$ for which due to the smoothness of ∂Z the estimate

$$\|\mathbf{v}_1\|_{L^2(\Omega^\varepsilon)} + \varepsilon \|\nabla \mathbf{v}_1\|_{L^2(\Omega^\varepsilon)} \lesssim \|q\|_{L^2(\Omega^\varepsilon)}$$

is valid. A second correction eliminates the wrong boundary values of $\mathbf{v}_1$ along Γ^ε: let $\mathbf{v}_2$ solve for each cell $Y^\varepsilon_{\mathbf{k}}$ with interior boundary $\Gamma^\varepsilon_{\mathbf{k}}$ a local Stokes problem with $\operatorname{div} \mathbf{v}_2 = 0$ and boundary values $\mathbf{v}_2 = -\mathbf{v_1}$ on $\Gamma^\varepsilon_{\mathbf{k}}$ and $\mathbf{v}_2 = 0$ on $\partial Y^\varepsilon_{\mathbf{k}} - \Gamma^\varepsilon_{\mathbf{k}}$. A scaling argument shows that

$$\|\nabla \mathbf{v}_2\|_{L^2(\Omega^\varepsilon, \mathbb{R}^n)} \lesssim \frac{1}{\varepsilon} \|\mathbf{v}_1\|_{L^2(\Omega, \mathbb{R}^n)} + \|\nabla \mathbf{v}_1\|_{L^2(\Omega, \mathbb{R}^n)} \lesssim \frac{1}{\varepsilon} \|q\|_{L^2(\Omega)} \,.$$

A third correction $\mathbf{v}_3$ is a boundary layer along $\partial\Omega$ which does not meet Γ^ε and corrects the boundary values of $\mathbf{v}_1$ along $\partial\Omega$. Since $\operatorname{dist}(\partial\Omega, \Gamma^\varepsilon) \gtrsim \varepsilon$, $\mathbf{v}_3$ can be shown to satisfy the same estimate as $\mathbf{v}_2$. Therefore, $\mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_3$ satisfies $\operatorname{div} \mathbf{v} = q$ and

$$\frac{(\operatorname{div} \mathbf{v}, q)_{L^2(\Omega^\varepsilon)}}{\|q\|_{L^2(\Omega^\varepsilon)} \|\mathbf{v}\|_{H^1_0(\Omega^\varepsilon, \mathbb{R}^n)}} \gtrsim \frac{\|q\|^2_{L^2(\Omega^\varepsilon)}}{\frac{1}{\varepsilon}\|q\|^2_{L^2(\Omega^\varepsilon)}} = \varepsilon$$

which proves (12). Finally, estimate (13) is an easy consequence of (11) and (12).

3 Homogenisation

The idea of homogenisation theory is that each of the problems presented in Section 2 allows, for small ε, the approximation by the solution of a certain homogenised problem without fine-scale features.

For problem (6),(7), the homogenised problem is to find $\mathbf{u}^0 \in H^1_0(\Omega, \mathbb{R}^n)$, such that

$$\mathbf{a}^0(\mathbf{u}^0, \mathbf{v}) := \int_\Omega \nabla \mathbf{v} : \mathbf{A}^0 \nabla \mathbf{u}^0 \, dx = \int_\Omega \mathbf{v} \cdot \mathbf{f} \, dx \,, \qquad \mathbf{v} \in H^1_0(\Omega, \mathbb{R}^n) \,. \tag{14}$$

where the matrix-valued homogenised tensor $\mathbf{A}^0 \in (\mathbb{R}^{n\times n})^{n\times n}$ is computed as

$$\mathbf{A}^0_{ij} = \int_\Box \left(\mathbf{A}_{ij}(y) + \sum_{l=1}^n \mathbf{A}_{il}(y) \frac{\partial \mathbf{N}_j}{\partial y_l}(y) \right) dy \tag{15}$$

with matrix-valued functions $\mathbf{N}_k \in H^1_{\mathrm{per},0}(\Box, \mathbb{R}^{n\times n})$, $k = 1, \ldots, n$ satisfying

$$\mathbf{a}(\mathbf{N}, \mathbf{v}) := \int_\Box \nabla \mathbf{v}(y) \mathbf{A}(y) \nabla \mathbf{N}_k(y) \, dy = -\int_\Box \nabla \mathbf{v}(y) \mathbf{A}(y) e_k \otimes \mathbf{I}^{n\times n} \, dy \tag{16}$$

for all $\mathbf{v} \in H^1_{\mathrm{per},0}(\Box, \mathbb{R}^n)$. It can be shown that $\mathbf{A}^0$ inherits ellipticity and continuity from $\mathbf{A}$, such that the Lemma of Lax-Milgram is again applicable and yields the existence of a unique solution $\mathbf{u}^0$ of (14).

Theorem 2. *Let* $\mathbf{u}^\varepsilon \in H_0^1(\Omega, \mathbb{R}^n)$ *be the solution of (6),* $\mathbf{N}_k \in H^1_{\text{per},0}(\square, \mathbb{R}^{n\times n})$ *be the solutions of (16), and* $\mathbf{u}^0 \in H_0^1(\Omega, \mathbb{R}^n)$ *be the solution of (14). Under the assumption* $u^0 \in H^2(\Omega)$ *the first-order corrector*

$$\mathbf{u}^{1,\varepsilon}(x) := \mathbf{u}^0(x) + \varepsilon \sum_{k=1}^n \mathbf{N}_k(\frac{x}{\varepsilon})\frac{\partial \mathbf{u}^0}{\partial x_k}(x) \in H^1(\Omega) \tag{17}$$

together with the boundary layer correction $\theta^\varepsilon \in u^{1,\varepsilon} + H_0^1(\Omega)$ *on* $\partial\Omega$ *and*

$$\int_\Omega \nabla \mathbf{v}^\varepsilon(x) : \mathbf{A}^\varepsilon(x) \nabla \theta^\varepsilon(x) dx = 0, \quad \mathbf{v}^\varepsilon \in H_0^1(\Omega) \tag{18}$$

satisfies the error estimate

$$\|\nabla(\mathbf{u}^\varepsilon - \mathbf{u}^{1,\varepsilon} - \theta^\varepsilon)\|_{L^2(\Omega)} \le C\varepsilon \|D^2 \mathbf{u}^0\|_{L^2(\Omega)}\,. \tag{19}$$

Furthermore, $\|\theta^\varepsilon\|_{H^1(\Omega)} \lesssim \varepsilon^{\frac{1}{2}}$ *and* $\|\theta^\varepsilon\|_{L^2(\Omega)} \lesssim \varepsilon$.

Proof. Although a similar estimate can be found in [10], it requires higher regularity of $\mathbf{u^0}$. Therefore, we give an alternative proof which follows [5],[9] for the diffusion case.

Since, for all $\mathbf{v} \in H_0^1(\Omega, \mathbb{R}^n)$,

$$\int_\Omega \nabla \mathbf{v} : \mathbf{A}^\varepsilon \nabla \mathbf{u}^\varepsilon \, dx = \int_\Omega \mathbf{v} \cdot \mathbf{f} \, dx = \int_\Omega \nabla \mathbf{v} : \mathbf{A}^0 \nabla \mathbf{u}^0 \, dx\,,$$

we have (note the renaming of the index k to j in a part of the expression in step 2)

$$\begin{aligned}
&\int_\Omega \nabla \mathbf{v} : \mathbf{A}^\varepsilon \nabla \Big(\mathbf{u}^\varepsilon - \mathbf{u}^0 - \varepsilon \sum_{k=1}^n \mathbf{N}_k(\frac{x}{\varepsilon}) \frac{\partial \mathbf{u}^0}{\partial x_k}\Big)\, dx = \\
&\quad \int_\Omega \nabla \frac{\partial \mathbf{v}}{\partial x_i} \Big(\mathbf{A}^0_{ij} \frac{\partial \mathbf{u}^0}{\partial x_j} - \mathbf{A}^\varepsilon_{ij} \frac{\partial \mathbf{u}^0}{\partial x_j} - \mathbf{A}^\varepsilon_{ij} \varepsilon \frac{\partial}{\partial x_j} (\sum_{k=1}^n \mathbf{N}_k(\frac{x}{\varepsilon}) \frac{\partial \mathbf{u}^0}{\partial x_k}) \Big)\, dx = \\
&\int_\Omega \frac{\partial \mathbf{v}}{\partial x_i} \big(\mathbf{A}^0_{ij} - \mathbf{A}^\varepsilon_{ij} - \mathbf{A}^\varepsilon_{ij} \nabla_y \mathbf{N}_j \big) \frac{\partial \mathbf{u}^0}{\partial x_j}\, dx + O(\varepsilon \|D^2 \mathbf{u}^0\|_{L^2(\Omega)} \|\nabla \mathbf{v}\|_{L^2(\Omega)})\,.
\end{aligned}$$

Now, because of the cell problems (16) each component of the matrix-valued tensor $\mathbf{T}_{ij} := \mathbf{A}^0_{ij} - \mathbf{A}_{ij} - \mathbf{A}_{ik} \frac{\partial \mathbf{N}_j}{\partial y_k}$ is divergence free with $\langle \mathbf{T}_{ij} \rangle_\square = 0$. By applying the subsequent Lemma 1 component-wise, there is a matrix-valued 3-tensor $\mathbf{S}^j_{ik}$ fulfilling $\mathbf{S}^j_{ik} = -\mathbf{S}^j_{ki}$ and $\sum_{k=1}^n \frac{\partial \mathbf{S}^j_{ik}}{\partial y_k} = \mathbf{T}_{ij}$. Since $\frac{\partial}{\partial y_k} = \varepsilon \frac{\partial}{\partial x_k}$, we have

$$\begin{aligned}
\int_\Omega \sum_{i,j=1}^n \frac{\partial \mathbf{v}}{\partial x_i} \mathbf{T}_{ij} \frac{\partial \mathbf{u}^0}{\partial x_j}\, dx &= \varepsilon \int_\Omega \sum_{i,j,k=1}^n \frac{\partial \mathbf{v}}{\partial x_i} \frac{\partial \mathbf{S}^j_{ik}}{\partial x_k} \frac{\partial \mathbf{u}^0}{\partial x_j}\, dx \\
&= \varepsilon \int_\Omega \sum_{i,j,k=1}^n \frac{\partial^2 \mathbf{v}}{\partial x_i \partial x_k} \mathbf{S}^j_{ik} \frac{\partial \mathbf{u}^0}{\partial x_j}\, dx + O(\varepsilon \|D^2 \mathbf{u}^0\|_{L^2(\Omega)} \|\nabla \mathbf{v}\|_{L^2(\Omega)})\,.
\end{aligned}$$

Due to the antisymmetry $\mathbf{S}^j_{ik} = -\mathbf{S}^j_{ki}$ the first term in the result vanishes, and the theorem is proved.

Lemma 1. *For* $1 < q < \infty$*, assume that the vector field* $\mathbf{t} \in L^q(\Box, \mathbb{R}^n)$ *satisfies* $\operatorname{div} \mathbf{t} = 0$ *in distributional sense together with* $\int_\Box \mathbf{t}\, dy = 0$*. Then there is a skew-symmetric matrix* $(S_{ik})_{i,k=1}^n \in (W^{1,q}(\Box))^{n\times n}$ *with*

$$\sum_{k=1}^n \frac{\partial S_{ik}}{\partial y_k} = t_i\,, \qquad i = 1, \ldots, n\,. \tag{20}$$

Proof. Define $S_{ik} = \frac{\partial \sigma_i}{\partial y_k} - \frac{\partial \sigma_k}{\partial y_i}$, where σ_i is the periodic solution of $\Delta \sigma_i = t_i$ on $\Box$ which exists because $\int_\Box t_i\, dy = 0$. It is easy to check that this S_{ik} satisfies all desired properties.

Finally, the homogenised problem for Stokes equation (9),(10) is the following Darcy problem. Given $\mathbf{f} \in L^2(\Omega, \mathbb{R}^n)$, and $g \in L^2_0(\Omega)$, we search for $p \in H^1(\Omega)$ and $u \in L^2(\Omega, \mathbb{R}^n)$ with $\operatorname{div} u \in L^2(\Omega)$ such that

$$\begin{aligned} \mathbf{u}(x) &= \mathbf{K}\left(\mathbf{f}(x) - \nabla p(x)\right) \quad \text{in } \Omega\,, \\ \operatorname{div} \mathbf{u}(x) &= g(x) \text{ in } \Omega\,, \\ \mathbf{u}\cdot\mathbf{n} &= 0 \text{ on } \partial\Omega\,. \end{aligned} \tag{21}$$

Here, the permeability tensor $\mathbf{K}$ is computed as

$$\mathbf{K}_{ij} = \int_Y (\nabla \mathbf{w}_i(y))^t \nabla \mathbf{w}_j(y)\, dy = \int_Y w_i^j(y)\, dy\,, \tag{22}$$

where, for $i = 1, \ldots, n$, the $(\mathbf{w}_i, \pi_i) \in H^1_{\text{per}}(Y, \mathbb{R}^n) \times L^2_0(Y)$ are weak solutions of the cell problems

$$\begin{aligned} -\Delta_y \mathbf{w}_i(y) + \nabla \pi_i(y) &= \mathbf{e}_i \quad \text{in } Y\,, \\ \operatorname{div} \mathbf{w}_i(y) &= 0 \quad \text{in } Y\,, \\ \mathbf{w}_i(y) &= 0 \quad \text{on } \partial Y\,. \end{aligned} \tag{23}$$

The following convergence result then links problem (9) with problem (21).

Theorem 3. *We assume that* g^ε *and* $\mathbf{f}^\varepsilon$ *are extended to* Ω *such that they converge strongly in* L^2 *to functions* $g \in L^2_0(\Omega)$ *and* $\mathbf{f} \in L^2(\Omega, \mathbb{R}^n)$ *for* $\varepsilon \to 0$*. Then the solutions* $\mathbf{u}^\varepsilon$ *of (9) (extended to* Ω *by 0) satisfy*

$$\frac{\mathbf{u}^\varepsilon}{\varepsilon^2} \rightharpoonup \mathbf{u} \quad (\varepsilon \to 0) \qquad\qquad \textit{weakly in } L^2(\Omega) \tag{24}$$

where $\mathbf{u}$ *denotes the solution to (21).*

Proof. The proof is a straightforward adaption of [11] where the divergence-free case $g \equiv 0$ was treated. $\Box$

Remark 1. In the divergence-free case, it is proved in [1] that $\frac{\mathbf{u}^\varepsilon}{\varepsilon^2}$ converges strongly in L^2 towards $\sum_{i=1}^n (f_i - \frac{\partial p}{\partial x_i})\mathbf{w}_i$. Furthermore, the error estimate $\|\frac{\mathbf{u}^\varepsilon}{\varepsilon^2} - \sum_{i=1}^n (f_i - \frac{\partial p}{\partial x_i})\mathbf{w}_i\|_{L^2(\Omega^\varepsilon)} \lesssim \varepsilon^{\frac{1}{6}}$ is proved in [6].

4 Numerical approximation of effective coefficients

In this section, we describe how to compute the effective coefficients (15) and (22) by solving the corresponding cell problems (16) and (23) numerically. Our method of choice are conforming finite element spaces of order p which allows for a good approximation of smooth problems, and a comparatively easy proof of error estimates.

For $h > 0$, let $T_h^{\square}$ denote a mesh of the unit cell $\square$ which fits across the identified boundary $\partial\square$. It has a set of cells $\mathcal{K}(T_h^{\square})$, where each cell $K \in \mathcal{K}(T_h^{\square})$ is an image of reference cells $\hat{K}_K$ under a smooth map $\Phi_K : \hat{K}_K \to K$. We consider only conforming meshes without hanging nodes. The reference cells $\hat{K}_K$ are allowed to be arbitrary products of unit-simplices of different dimensions, which allows both simplex and cube meshes as a special cases. We ensure a reasonable quality of $T_h^{\square}$ by assuming that there is some $d_T \in \mathbb{N}, d_T \geq 2$ and some constant $C_T > 0$ such that for all cells $K \in T_h^{\square}$ with associated map $\Phi_K : \hat{K} \to K$ to its reference cell $\hat{K}$, we have

$$\|D^\alpha \Phi_K\|_{L^\infty(\hat{K})} \leq C_T h^{|\alpha|}\,, \qquad \forall \alpha : 0 \leq |\alpha| \leq d_T \tag{25}$$

$$\|\Phi_K^{-1}\|_{C^{0,1}(K)} \leq C_T h^{-1}\,. \tag{26}$$

For $1 \leq p \leq d_T - 1$, we now define conforming finite element spaces of order $p \in \mathbb{N}$ on T_h. Writing a reference cell $\hat{K} = s_1 \times \cdots \times s_l$ as a product of simplices of dimensions $d_1, \ldots, d_l$, we define

$$S^p(\hat{K}) = \{p = p_1 \otimes \ldots \otimes p_l : p_i \in P^p(s_i)\} \tag{27}$$

as the space of polynomials which are tensor products of polynomials on the factor simplices s_i with degree p. This is used to define the following finite element spaces

$$S^p(T_h^{\square}) = \{\varphi \in H^1(\square) : \forall K \in \mathcal{K}(T_h^{\square}) : \varphi \circ \Phi_K \in S^p(\hat{K}_K)\}\,, \tag{28}$$

$$S^p_{\mathrm{per}}(T_h^{\square}) = S^p(T_h^{\square}) \cap H^1_{\mathrm{per}}(\square)\,, \qquad S^p_{\mathrm{per},0} = S^p_{\mathrm{per}} \cap L^2_0(\square)\,. \tag{29}$$

Analogous to the notation of function spaces, vector-valued finite element spaces are denoted as $S^p(T_h^{\square}, \mathbb{R}^n) \cong (S^p(T_h^{\square}))^n$, etc.

For computing the effective elastic tensor (15) we then have the following approximation result.

Theorem 4. *Let* $\mathbf{N}_h \in S^p_{\mathrm{per},0}(T_h^{\square}, \mathbb{R}^{n^3})$ *denote the finite element approximation of the tensor* $\mathbf{N}$ *from problem (16). Then, for all* $1 \leq k \leq p$, *we have the error estimate*

$$\|\nabla(\mathbf{N} - \mathbf{N}_h)\|_{L^2(\square)} \leq C(n, p, C_T) h^k \|\mathbf{N}\|_{H^{k+1}(\square)}\,. \tag{30}$$

Computing the homogenised coefficients using $\mathbf{N}_h$ *instead of* $\mathbf{N}$ *in formula (15) then yields an approximation* $\mathbf{A}^0_h$ *which satisfies*

$$\|\mathbf{A}^0_h - \mathbf{A}^0\|_\infty \lesssim h^{2k}\,. \tag{31}$$

Proof. (30) is a consequence of standard finite element approximation theory. Inequality (31) follows because

$$\mathbf{A}_h^0 - \mathbf{A}^0 = \int_\Box \mathbf{A}(y)\nabla(\mathbf{N}_h - \mathbf{N}) = \int_\Box \nabla\mathbf{N}\mathbf{A}(y)\nabla(\mathbf{N} - \mathbf{N}_h)$$

and due to Galerkin orthogonality

$$\int_\Box \nabla\mathbf{N}\mathbf{A}(y)\nabla(\mathbf{N} - \mathbf{N}_h) = \int_\Box \nabla(\mathbf{N} - \mathbf{N}_h)\mathbf{A}(y)\nabla(\mathbf{N} - \mathbf{N}_h) \lesssim h^{2k}\,.$$

□

For discretising the Stokes cell problems (23) we use again finite elements on a mesh T_h^Y of the cell Y. Our method of choice are Taylor-Hood elements of order p, where

$$\mathbf{V}_h = \{\mathbf{v} \in S_{\mathrm{per}}^{p+1}(T_h^Y, \mathbb{R}^n) : \mathbf{v} = 0 \text{ on } \Gamma\} \tag{32}$$

and

$$\Pi_h = L_0^2(Y) \cap S_{\mathrm{per}}^p(T_h^Y) \tag{33}$$

are ansatz spaces for velocity, resp. pressure. For $p \geq 1$ and under mild assumptions on T_h^Y, this pair of spaces is known to be stable uniformly in h, see [3]. An immediate consequence is the following error estimate:

Theorem 5. *Let $\mathbf{w}_{i,h} \in \mathbf{V}_h, \pi_{i,h} \in \Pi_h$ be the finite element solution of (9). If $\mathbf{w}_i \in H^{k+1}(Y)$ and $\pi_i \in H^k(Y)$ for some $1 \leq k \leq p$, then*

$$\|\nabla(\mathbf{w}_i - \mathbf{w}_{i,h})\|_{L^2(Y)} + h\|\nabla(\pi_i - \pi_{i,h})\|_{L^2(Y)} \lesssim h^k(\|\mathbf{w}_i\|_{H^{k+1}(Y)} + \|\pi_i\|_{H^k(Y)})\,. \tag{34}$$

If problem (23) is H^2-regular, we have also

$$\|\mathbf{w}_i - \mathbf{w}_{i,h}\|_{L^2(Y)} + h\|\pi_i - \pi_{i,h}\|_{L^2(Y)} \lesssim h^{k+1}(\|\mathbf{w}_i\|_{H^{k+1}(Y)} + \|\pi_i\|_{H^k(Y)})\,. \tag{35}$$

The components of the permeability $\mathbf{K}$ are obtained as the right-hand sides of (23) evaluated on the solutions $\mathbf{w}_i$, such that we obtain in a similar way to the proof of Theorem 4 the following estimate.

Corollary 1. *Using the finite element solutions $\mathbf{w}_{i,h}$ in formula (22) leads to an approximation $\mathbf{K}_h$ of $\mathbf{K}$. Under the assumption of H^2-regularity of the cell problems (23), and if for some $1 \leq k \leq p$ we have $\mathbf{w}_i \in H^{k+1}(\Omega, \mathbb{R}^n)$, $\pi_i \in H^k(\Omega)$ for $i = 1, \ldots, n$, then*

$$\|\mathbf{K} - \mathbf{K}_h\|_\infty \lesssim h^{2k}\,. \tag{36}$$

Remark 2. Of course, high regularity of the cell solutions $\mathbf{N}_i$ (resp. $\mathbf{w}_i$ and π_i) can only be expected, if the elasticity tensor $\mathbf{A}$ (resp. the pore boundary ∂Z) are sufficiently smooth. If this is not the case, mesh adaption becomes necessary, and a more sophisticated error analysis has to be performed, cf. [12], [2].

5 Numerical results

In this section, we first demonstrate the high-accuracy calculation of effective coefficients corresponding to Section 4. Then we demonstrate the use of effective equations for constructing optimal preconditioners. All calculations in this section were done with the object-oriented interactive finite element toolbox Femlisp, see [7], [4]. More information can be found in [8].

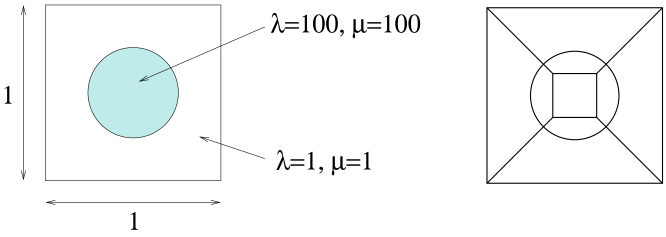

Fig. 1. Lamé constants and coarsest mesh.

First, we want to calculate the effective coefficient for two-dimensional linear elasticity where the isotropic elasticity tensor

$$A_{ij}^{kl}(x) = \lambda(x)\delta_{ik}\delta_{jl} + \mu(x)(\delta_{ij}\delta_{kl} + \delta_{kj}\delta_{il}) \tag{37}$$

is determined by the Lamé parameters $\lambda, \mu > 0$ and describes a circular inlay, see the left-hand side of Fig. 1. The right-hand side of Fig. 1 shows the coarsest mesh which resolves the inlay exactly.[1] This coarse mesh is then uniformly refined to yield improved approximations. Using a polynomial degree $p = 5$ for approximating the tensor $\mathbf{N}$ as described in Section 4, we obtain the following results for approximating $\mathbf{A}^0$:

N_{cell}	N_{dof}	N_{entries}	CPU	A_{11}^{11}	A_{12}^{12}	A_{12}^{21}
9	1800	43060	5.4	4.1458940638	1.3176717343	1.2966840277
36	7200	176224	23.7	4.1412496929	1.3139564023	1.2979726371
144	28800	705600	74.9	4.1412384319	1.3139473004	1.2979716831
576	115200	2822400	293.8	4.1412383854	1.3139472825	1.2979716903

Here N_{cell} denotes the number of cells, N_{dof} denotes the number of the degrees of freedom, N_{entries} denotes the number of matrix entries, and CPU gives the number of seconds the calculation needed on a PC (2.4 GHz Pentium 4 processor, 1 Gigabyte main memory). The last three columns give three components of the effective tensor $\mathbf{A}_h^0$ which uniquely determine the

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[1] An isoparametric approximation of the interface would have led to a suboptimal order of convergence because the integration of $\mathbf{A}$ over cells occurring in (15) would not have been calculated accurately enough.

whole tensor due to symmetry properties. We observe a very fast convergence which is in accordance with the theoretical estimate of Theorem 4. Note that this elasticity tensor does not describe an isotropic elastic medium in spite of the Cartesian symmetry of the cell.

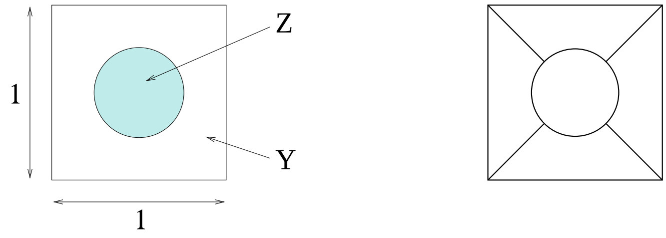

Fig. 2. Porous cell and coarsest mesh.

Next, we consider the calculation of a permeability tensor as described in Section 4. We consider the two-dimensional geometry shown in Fig. 2 We use the pair $\mathbf{V}_h \times \Pi_h$ from (32), (33) for $p = 4$ and obtain the following results:

N_{cell}	N_{dof}	N_{entries}	CPU	K
4	578	33823	1.2	1.9943087655d-02
16	2218	142179	12.2	1.9901508352d-02
64	8666	567991	41.0	1.9901435210d-02
256	34234	2267511	158.5	1.9901435350d-02

Also in this case we observe a rapid convergence which is in accordance with Theorem 5. Note that because of the symmetric geometry, the permeability is actually a scalar multiple of the identity. Fig. 3 shows the solution $(\mathbf{w}_i, \pi_i)$ for $i = 1$ (first row) and $i = 2$ (second row).

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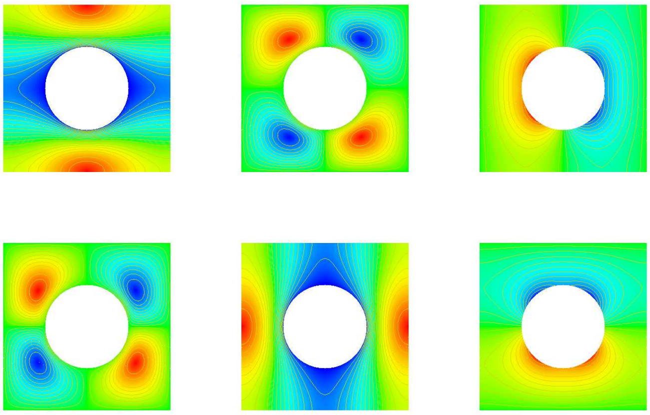

Fig. 3. Solutions $\mathbf{w_i}, \pi_i$ of (23).

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